



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:54 AM UTC

PDB ID : 1H8H / pdb_00001h8h
Title : Bovine mitochondrial F1-ATPase crystallised in the presence of 5mm AMPPNP
Authors : Braig, K.; Menz, R.I.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2001-02-06
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

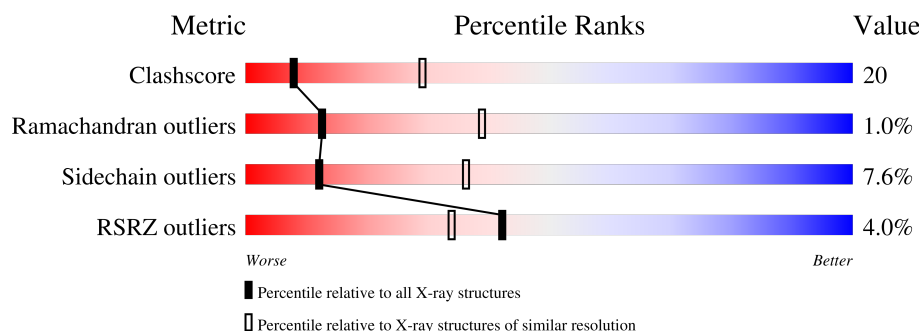
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	510	2% 53% 36% 5% • 5%
1	B	510	3% 49% 38% 6% 6%
1	C	510	2% 54% 36% 6% • •
2	D	482	4% 55% 37% • • •
2	E	482	5% 49% 43% • • •
2	F	482	2% 57% 34% 5% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	272	9% 26% 15% 50%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22941 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	engineered mutation	UNP P19483
B	481	GLY	SER	engineered mutation	UNP P19483
C	481	GLY	SER	engineered mutation	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			

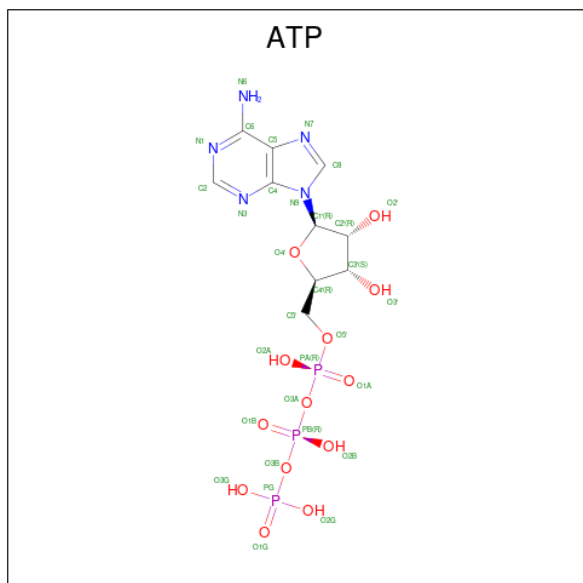
- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	43	VAL	ILE	engineered mutation	UNP P05631

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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

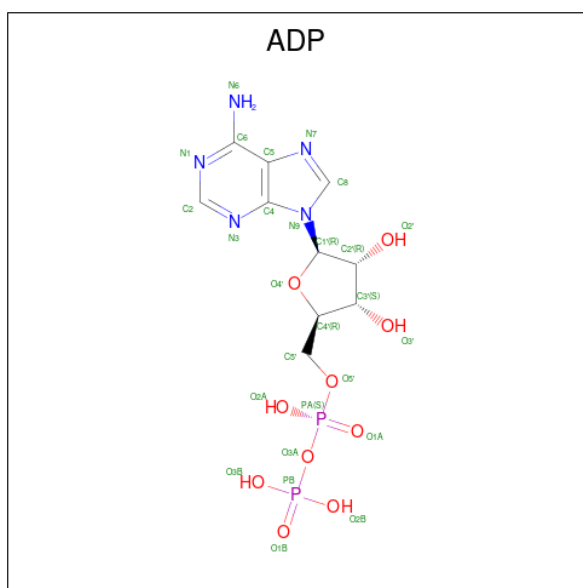
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

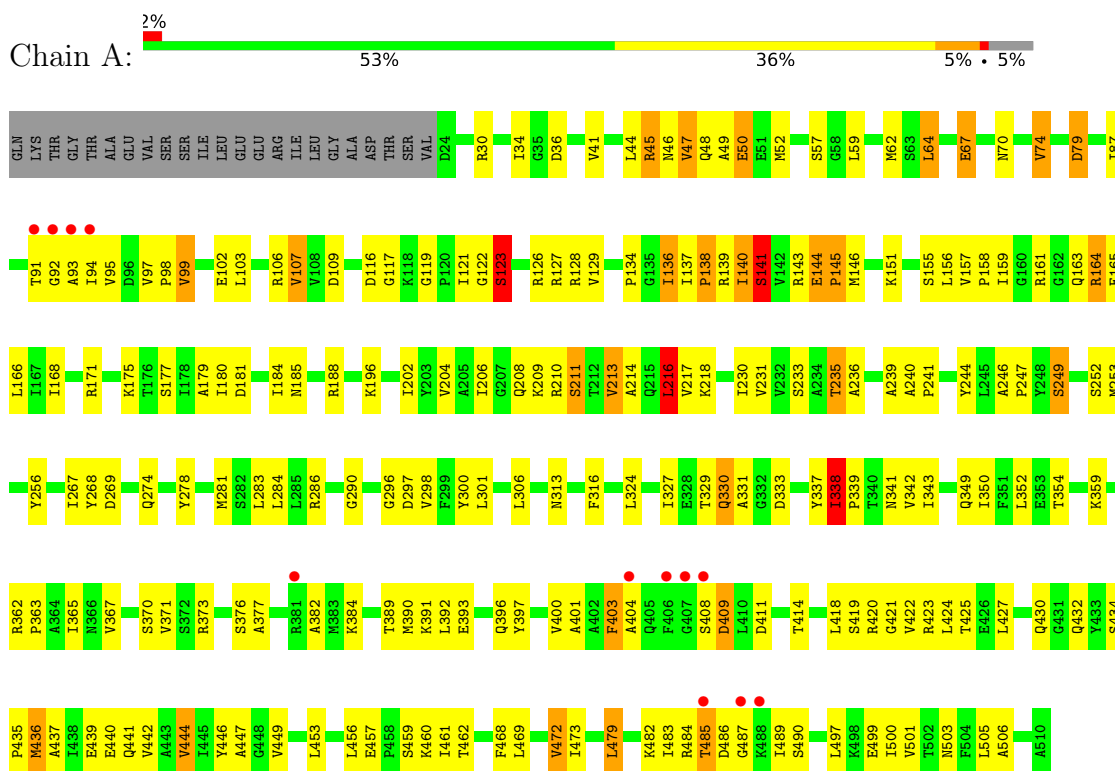
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	24	Total	O	0	0
			24	24		
9	B	26	Total	O	0	0
			26	26		
9	C	14	Total	O	0	0
			14	14		
9	D	15	Total	O	0	0
			15	15		
9	E	13	Total	O	0	0
			13	13		
9	F	17	Total	O	0	0
			17	17		
9	G	2	Total	O	0	0
			2	2		

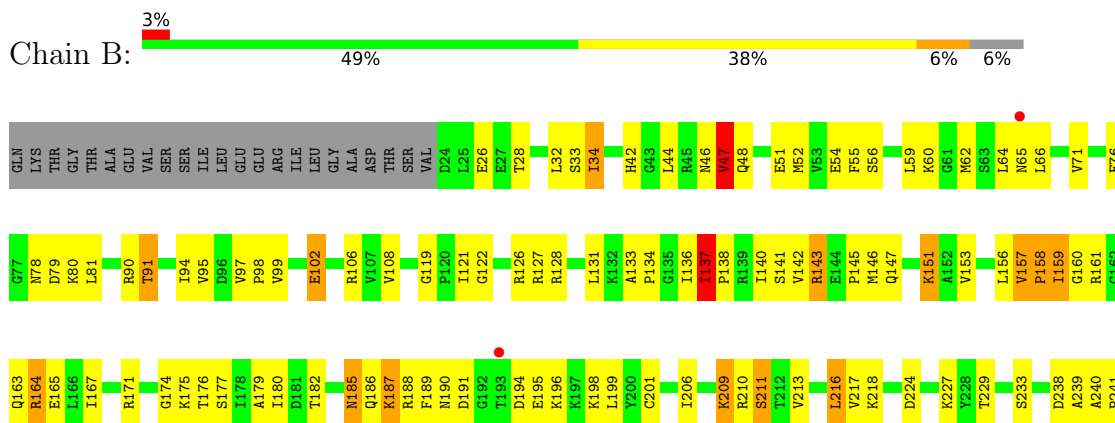
3 Residue-property plots [i](#)

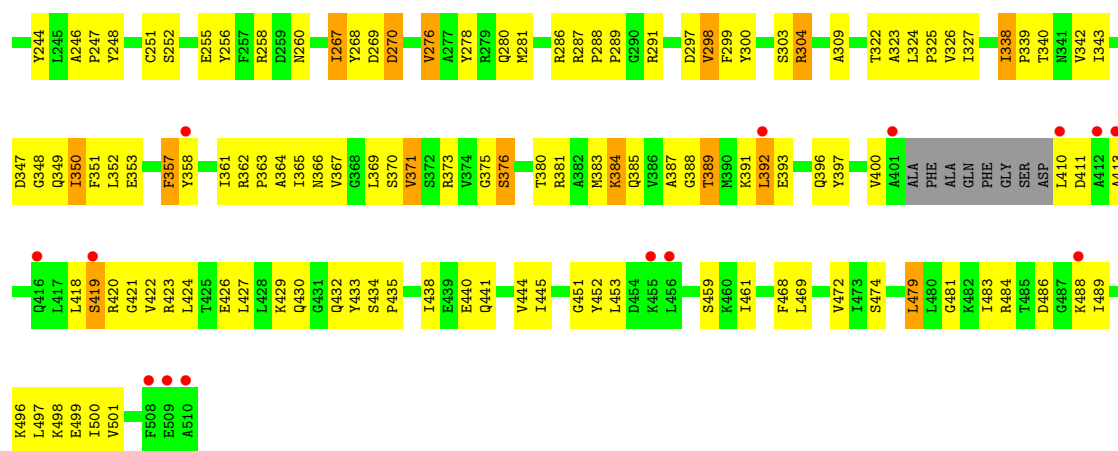
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

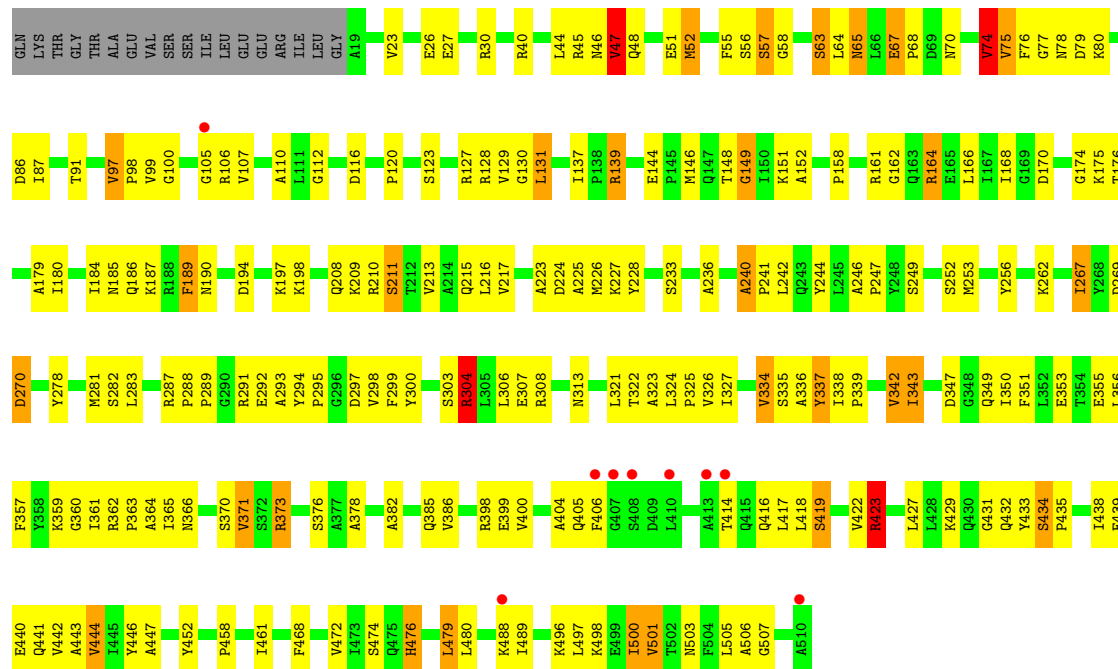


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

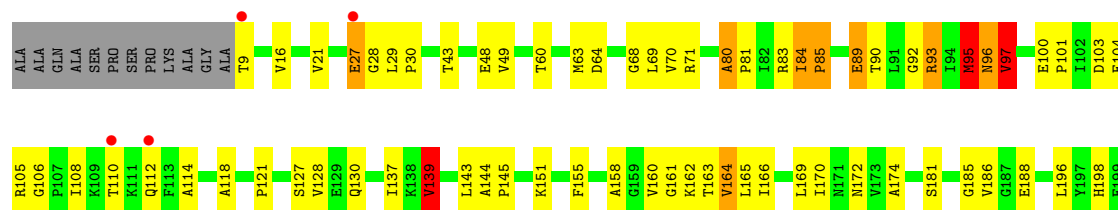


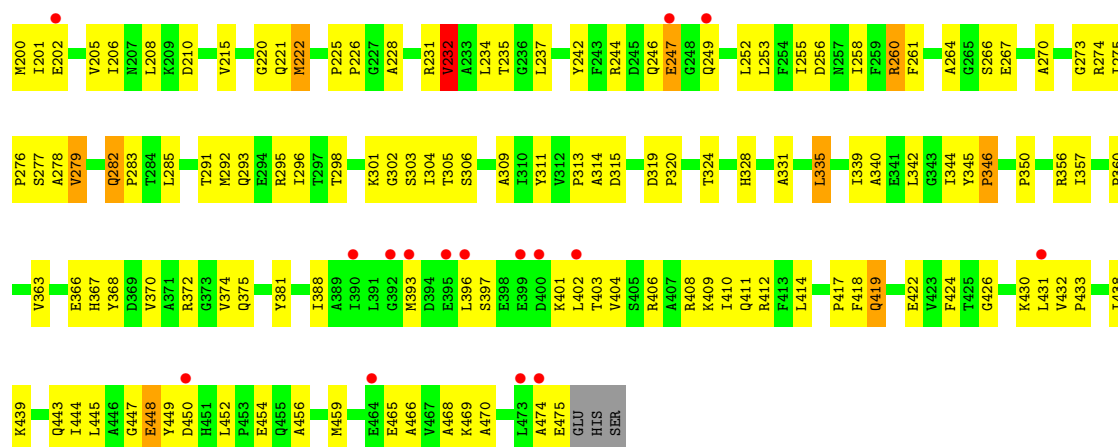


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

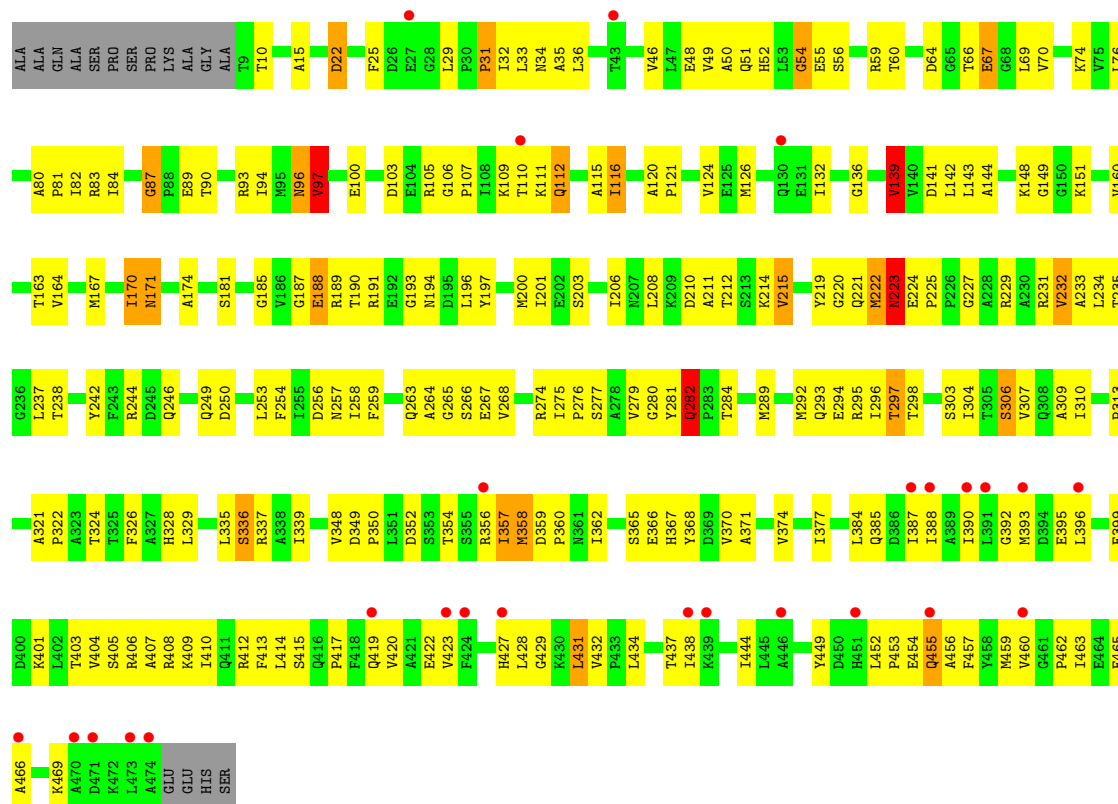


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



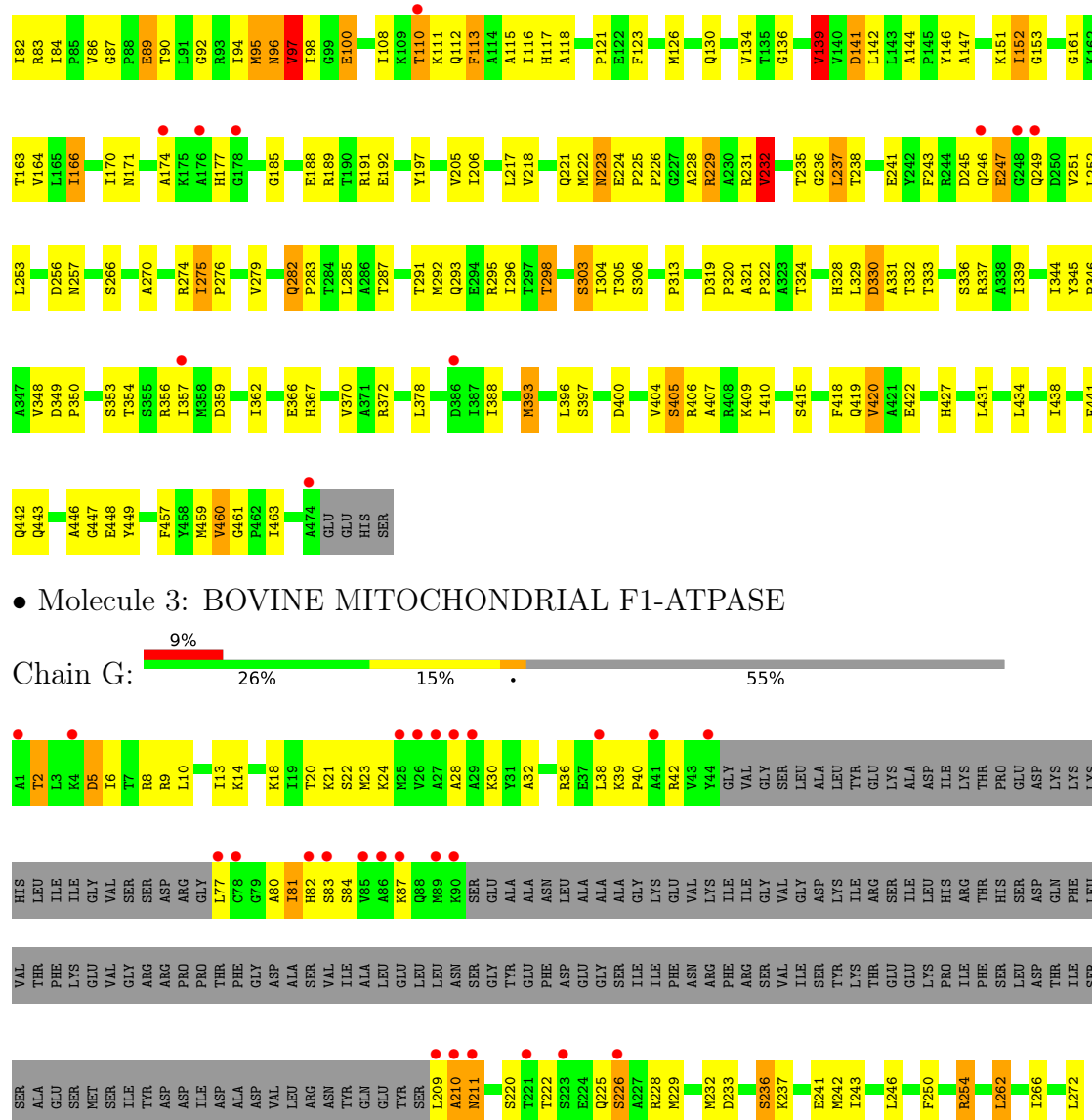


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	280.00Å 107.00Å 139.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-2.90) 96.3 (20.00-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.37 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.292 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22941	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4, ATP, GOL, ADP

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	0.68	0/3766	1.57	43/5080 (0.8%)
1	B	0.70	0/3704	1.55	43/4995 (0.9%)
1	C	0.73	0/3799	1.64	45/5126 (0.9%)
2	D	0.71	0/3596	1.63	49/4879 (1.0%)
2	E	0.64	0/3587	1.52	40/4867 (0.8%)
2	F	0.73	0/3587	1.62	60/4867 (1.2%)
3	G	0.56	0/949	1.23	1/1266 (0.1%)
All	All	0.69	0/22988	1.57	281/31080 (0.9%)

There are no bond length outliers.

All (281) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	97	VAL	CB-CA-C	-11.40	97.38	111.97
1	C	373	ARG	CD-NE-CZ	11.27	140.18	124.40
2	D	139	VAL	CB-CA-C	-9.69	99.47	111.88
2	F	171	ASN	CA-CB-CG	8.61	121.21	112.60
2	E	97	VAL	CB-CA-C	-8.57	100.91	111.88
2	F	139	VAL	CB-CA-C	-8.51	100.81	111.70
2	D	139	VAL	N-CA-CB	8.38	119.81	110.51
2	D	260	ARG	NE-CZ-NH2	8.26	126.63	119.20
1	B	136	ILE	CA-C-N	8.06	126.78	120.33
1	B	136	ILE	C-N-CA	8.06	126.78	120.33
2	D	96	ASN	OD1-CG-ND2	7.82	130.42	122.60
2	E	223	ASN	CA-CB-CG	7.68	120.28	112.60
2	D	95	MET	CA-C-N	7.68	136.53	122.02
2	D	95	MET	C-N-CA	7.68	136.53	122.02
2	E	359	ASP	CA-CB-CG	7.55	120.15	112.60
2	F	86	VAL	CA-C-O	-7.52	113.93	121.45
2	E	139	VAL	CB-CA-C	-7.45	99.08	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	VAL	CB-CA-C	-7.36	101.79	111.13
1	C	164	ARG	CD-NE-CZ	7.30	134.63	124.40
2	D	344	ILE	CA-C-O	-7.25	112.18	120.74
1	C	476	HIS	CA-CB-CG	-7.19	106.61	113.80
1	A	92	GLY	CA-C-N	7.18	135.26	121.54
1	A	92	GLY	C-N-CA	7.18	135.26	121.54
1	A	106	ARG	CD-NE-CZ	7.12	134.37	124.40
1	C	139	ARG	NE-CZ-NH1	-7.10	114.40	121.50
1	C	75	VAL	CA-C-O	-7.02	113.04	121.04
1	B	185	ASN	CA-CB-CG	6.99	119.59	112.60
2	D	103	ASP	CA-CB-CG	6.96	119.56	112.60
2	E	432	VAL	CA-C-O	6.93	123.24	119.15
1	B	136	ILE	N-CA-C	6.93	117.08	110.42
2	F	189	ARG	NE-CZ-NH1	-6.91	114.59	121.50
2	F	189	ARG	NE-CZ-NH2	6.91	125.42	119.20
1	B	357	PHE	CA-CB-CG	6.91	120.71	113.80
2	E	282	GLN	CA-C-N	6.89	127.18	119.32
2	E	282	GLN	C-N-CA	6.89	127.18	119.32
2	E	233	ALA	N-CA-C	-6.87	103.79	111.28
1	C	429	LYS	CA-C-O	-6.83	113.76	121.81
1	B	298	VAL	N-CA-CB	6.82	122.30	110.65
1	A	74	VAL	N-CA-CB	-6.78	103.27	111.21
1	C	144	GLU	CA-C-O	6.78	124.68	119.46
2	D	419	GLN	CA-C-O	6.72	128.09	120.90
2	D	97	VAL	N-CA-CB	6.72	118.41	110.55
1	C	423	ARG	CD-NE-CZ	6.71	133.79	124.40
2	E	349	ASP	CA-C-N	6.71	126.33	119.56
2	E	349	ASP	C-N-CA	6.71	126.33	119.56
1	B	164	ARG	CA-C-O	-6.67	113.17	120.30
2	D	90	THR	N-CA-C	-6.67	105.30	113.50
1	B	71	VAL	CA-C-N	-6.66	115.87	122.20
1	B	71	VAL	C-N-CA	-6.66	115.87	122.20
1	C	74	VAL	N-CA-CB	-6.62	103.12	111.46
2	E	432	VAL	CA-C-N	6.60	126.51	119.85
2	E	432	VAL	C-N-CA	6.60	126.51	119.85
2	F	100	GLU	CB-CG-CD	-6.60	101.39	112.60
2	D	261	PHE	CA-CB-CG	6.57	120.37	113.80
2	D	275	ILE	N-CA-C	-6.53	102.95	109.02
2	D	95	MET	CA-C-O	6.48	129.57	121.66
1	B	349	GLN	CA-CB-CG	6.45	127.01	114.10
2	D	222	MET	CB-CA-C	-6.44	96.73	110.32
2	F	298	THR	CA-C-O	-6.43	114.22	121.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	83	ARG	CD-NE-CZ	6.40	133.37	124.40
1	C	240	ALA	CA-C-O	6.35	124.47	118.63
2	F	41	ARG	CG-CD-NE	6.35	125.98	112.00
1	B	153	VAL	N-CA-C	6.34	116.49	110.53
2	F	90	THR	N-CA-C	-6.33	105.86	113.97
1	C	233	SER	N-CA-C	6.33	118.83	108.52
1	B	270	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	144	GLU	CA-C-N	6.32	126.53	119.90
1	A	144	GLU	C-N-CA	6.32	126.53	119.90
2	F	337	ARG	NE-CZ-NH2	6.32	124.88	119.20
1	A	236	ALA	N-CA-C	6.30	118.96	111.33
1	B	189	PHE	CA-CB-CG	6.30	120.10	113.80
2	F	304	ILE	CB-CA-C	-6.30	101.56	110.12
1	B	298	VAL	CB-CA-C	-6.29	102.41	112.16
2	F	330	ASP	CA-CB-CG	-6.28	106.32	112.60
2	E	96	ASN	CA-CB-CG	6.27	118.87	112.60
2	F	96	ASN	CA-CB-CG	6.26	118.86	112.60
2	F	87	GLY	CA-C-N	6.24	126.15	119.28
2	F	87	GLY	C-N-CA	6.24	126.15	119.28
2	D	84	ILE	N-CA-CB	6.24	116.97	111.67
1	C	58	GLY	N-CA-C	-6.23	107.28	114.69
2	D	298	THR	N-CA-C	-6.23	102.31	110.53
2	E	22	ASP	CA-CB-CG	6.20	118.80	112.60
2	E	232	VAL	CA-C-O	-6.20	113.04	120.78
1	A	171	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	A	52	MET	CA-C-O	-6.18	113.41	120.58
1	A	306	LEU	N-CA-C	6.16	119.63	111.75
2	F	59	ARG	CA-C-O	-6.15	113.85	120.92
1	C	158	PRO	CA-C-O	-6.14	114.66	121.23
1	A	269	ASP	CA-CB-CG	6.13	118.73	112.60
1	C	223	ALA	CA-C-O	6.11	126.45	119.18
2	E	54	GLY	CA-C-O	-6.09	118.26	122.22
2	D	64	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	425	THR	O-C-N	6.08	128.42	122.09
1	B	137	ILE	CA-C-O	6.08	122.76	118.69
1	C	97	VAL	N-CA-C	6.04	114.15	109.19
1	C	75	VAL	N-CA-C	6.04	116.85	109.30
1	B	370	SER	CA-C-O	-6.01	114.56	121.47
2	F	97	VAL	CB-CA-C	-6.00	101.45	111.29
1	C	67	GLU	CA-C-N	5.99	125.70	119.05
1	C	67	GLU	C-N-CA	5.99	125.70	119.05
2	D	221	GLN	N-CA-C	5.98	117.61	110.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	225	PRO	N-CA-CB	5.97	106.53	103.19
2	F	275	ILE	N-CA-C	-5.97	103.10	108.95
2	E	225	PRO	CA-C-N	5.94	126.09	119.32
2	E	225	PRO	C-N-CA	5.94	126.09	119.32
1	A	274	GLN	N-CA-C	-5.92	104.90	111.36
1	B	338	ILE	CA-C-O	5.92	122.66	118.69
1	B	371	VAL	CB-CA-C	-5.92	101.23	110.52
2	D	301	LYS	N-CA-C	5.91	117.80	111.36
2	E	432	VAL	N-CA-C	5.89	113.71	107.76
2	F	313	PRO	N-CA-CB	5.89	108.55	103.36
1	C	47	VAL	N-CA-CB	5.89	120.02	110.13
2	F	144	ALA	CA-C-N	5.89	125.89	119.89
2	F	144	ALA	C-N-CA	5.89	125.89	119.89
2	D	93	ARG	NE-CZ-NH2	-5.87	113.92	119.20
2	D	105	ARG	CD-NE-CZ	5.84	132.57	124.40
2	E	64	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	137	ILE	N-CA-C	5.83	119.34	112.35
2	D	273	GLY	O-C-N	-5.83	116.03	122.50
1	B	309	ALA	N-CA-C	-5.82	101.00	110.20
1	A	290	GLY	CA-C-O	-5.81	116.49	121.78
1	A	338	ILE	N-CA-CB	5.81	114.16	110.50
1	C	47	VAL	CB-CA-C	-5.79	101.88	111.32
1	A	338	ILE	CB-CG1-CD1	5.78	125.94	113.80
1	A	163	GLN	OE1-CD-NE2	-5.77	116.83	122.60
1	C	343	ILE	CB-CA-C	-5.77	104.48	112.04
2	E	171	ASN	OD1-CG-ND2	5.77	128.37	122.60
2	D	232	VAL	N-CA-C	5.76	116.41	110.36
2	F	30	PRO	CA-C-N	5.74	125.69	119.78
2	F	30	PRO	C-N-CA	5.74	125.69	119.78
2	D	225	PRO	CA-C-N	5.73	125.20	119.24
2	D	225	PRO	C-N-CA	5.73	125.20	119.24
1	A	216	LEU	CA-CB-CG	5.73	136.34	116.30
2	D	426	GLY	N-CA-C	-5.72	105.03	114.76
1	A	337	TYR	N-CA-C	5.72	117.20	110.97
2	F	256	ASP	CA-CB-CG	5.71	118.31	112.60
2	F	256	ASP	CA-C-N	5.70	131.95	121.70
2	F	256	ASP	C-N-CA	5.70	131.95	121.70
2	F	331	ALA	CA-C-O	-5.70	113.77	120.60
1	B	213	VAL	CA-C-N	5.68	128.20	120.54
1	B	213	VAL	C-N-CA	5.68	128.20	120.54
1	B	348	GLY	CA-C-O	-5.67	117.51	122.16
1	A	164	ARG	N-CA-CB	5.66	119.60	110.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	419	GLN	CA-C-N	5.66	130.03	120.64
2	F	419	GLN	C-N-CA	5.66	130.03	120.64
2	D	139	VAL	N-CA-C	5.65	116.30	110.36
1	C	236	ALA	N-CA-C	5.65	118.16	111.33
1	C	91	THR	CA-C-O	5.64	125.01	118.97
2	F	152	ILE	CA-C-N	-5.64	118.21	122.33
2	F	152	ILE	C-N-CA	-5.64	118.21	122.33
1	A	403	PHE	CA-CB-CG	5.62	119.42	113.80
3	G	254	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	B	267	ILE	CA-C-O	-5.59	114.58	120.39
2	E	277	SER	N-CA-CB	5.59	119.75	110.14
1	A	107	VAL	N-CA-CB	5.59	118.90	111.64
1	C	120	PRO	N-CA-CB	5.57	108.00	103.32
1	B	126	ARG	CD-NE-CZ	5.56	132.18	124.40
1	C	47	VAL	O-C-N	5.55	128.51	122.63
2	E	87	GLY	CA-C-N	5.54	126.77	119.84
2	E	87	GLY	C-N-CA	5.54	126.77	119.84
2	F	350	PRO	N-CA-CB	5.54	108.62	103.41
1	C	350	ILE	CA-C-O	-5.54	114.31	120.74
2	D	96	ASN	CB-CA-C	-5.54	99.59	111.78
2	F	303	SER	CA-C-N	5.54	131.17	122.70
2	F	303	SER	C-N-CA	5.54	131.17	122.70
2	D	302	GLY	CA-C-N	-5.53	114.64	122.94
2	D	302	GLY	C-N-CA	-5.53	114.64	122.94
1	B	276	VAL	N-CA-CB	5.53	118.87	110.58
1	A	233	SER	N-CA-C	5.53	117.42	108.41
2	F	191	ARG	CA-CB-CG	5.52	125.15	114.10
2	F	232	VAL	CA-C-O	-5.51	113.89	120.78
1	A	91	THR	CA-C-N	5.50	132.18	121.41
1	A	91	THR	C-N-CA	5.50	132.18	121.41
1	A	138	PRO	N-CA-CB	5.50	108.69	103.19
1	A	327	ILE	CA-C-O	5.48	126.40	120.43
2	F	226	PRO	N-CA-CB	5.48	109.00	103.25
1	A	434	SER	CA-C-N	5.46	125.73	119.83
1	A	434	SER	C-N-CA	5.46	125.73	119.83
2	D	96	ASN	N-CA-CB	-5.46	102.13	110.49
2	F	113	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	46	ASN	CA-CB-CG	5.45	118.05	112.60
2	D	276	PRO	N-CA-CB	5.45	108.09	103.35
2	E	54	GLY	N-CA-C	-5.45	106.78	111.95
2	F	139	VAL	N-CA-CB	5.43	116.32	110.62
1	C	500	ILE	N-CA-C	5.42	116.15	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	PRO	N-CA-CB	5.42	108.13	103.31
1	C	507	GLY	N-CA-C	-5.42	106.09	112.64
1	C	57	SER	N-CA-C	5.41	119.50	113.01
2	E	222	MET	CA-C-O	-5.41	113.99	120.10
2	E	96	ASN	N-CA-CB	-5.39	102.73	110.44
2	E	244	ARG	CD-NE-CZ	5.39	131.95	124.40
2	E	336	SER	N-CA-C	5.38	117.85	108.76
1	C	304	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	B	238	ASP	CA-CB-CG	-5.37	107.23	112.60
1	C	75	VAL	CB-CA-C	-5.36	103.34	111.33
1	A	67	GLU	CA-C-N	5.35	124.81	119.24
1	A	67	GLU	C-N-CA	5.35	124.81	119.24
2	D	226	PRO	N-CA-CB	5.35	108.99	103.15
2	E	274	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	B	157	VAL	CA-C-N	5.34	126.52	119.84
1	B	157	VAL	C-N-CA	5.34	126.52	119.84
2	D	344	ILE	O-C-N	5.33	128.81	122.83
2	F	353	SER	CA-C-O	-5.33	114.62	120.43
1	B	119	GLY	CA-C-N	5.33	125.30	120.03
1	B	119	GLY	C-N-CA	5.33	125.30	120.03
2	E	90	THR	N-CA-C	-5.33	106.62	113.23
1	C	386	VAL	N-CA-C	5.32	115.53	110.53
2	E	97	VAL	N-CA-C	5.32	115.94	110.36
1	C	149	GLY	N-CA-C	-5.31	107.99	115.32
1	C	106	ARG	CA-CB-CG	-5.31	103.48	114.10
2	E	144	ALA	CA-C-N	5.29	125.55	119.83
2	E	144	ALA	C-N-CA	5.29	125.55	119.83
2	F	19	ALA	CA-C-N	-5.29	116.25	123.12
2	F	19	ALA	C-N-CA	-5.29	116.25	123.12
1	A	300	TYR	CA-CB-CG	5.28	123.39	113.90
2	D	144	ALA	CA-C-N	5.27	125.19	119.76
2	D	144	ALA	C-N-CA	5.27	125.19	119.76
2	D	344	ILE	CB-CA-C	-5.26	104.92	111.08
1	C	434	SER	CA-C-N	5.26	125.26	119.90
1	C	434	SER	C-N-CA	5.26	125.26	119.90
1	A	145	PRO	N-CA-CB	5.24	107.97	103.36
2	D	273	GLY	CA-C-O	5.24	124.62	118.96
2	F	90	THR	CA-C-O	5.23	124.56	118.97
1	B	91	THR	N-CA-C	-5.22	106.94	113.72
2	F	225	PRO	CA-C-N	5.20	126.34	119.84
2	F	225	PRO	C-N-CA	5.20	126.34	119.84
2	D	346	PRO	N-CA-CB	5.20	108.32	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	67	GLU	CA-CB-CG	5.20	124.50	114.10
1	A	341	ASN	OD1-CG-ND2	-5.19	117.41	122.60
2	D	185	GLY	N-CA-C	-5.19	100.88	113.18
2	F	185	GLY	CA-C-N	-5.19	116.20	123.10
2	F	185	GLY	C-N-CA	-5.19	116.20	123.10
1	B	433	TYR	CA-C-N	-5.18	116.84	122.59
1	B	433	TYR	C-N-CA	-5.18	116.84	122.59
2	D	331	ALA	CA-C-O	-5.18	114.16	120.54
1	C	342	VAL	CA-C-O	-5.18	115.30	121.05
1	B	145	PRO	N-CA-CB	5.18	107.93	103.27
2	D	424	PHE	CA-CB-CG	5.17	118.97	113.80
1	C	184	ILE	CA-C-N	5.17	127.21	120.28
1	C	184	ILE	C-N-CA	5.17	127.21	120.28
2	F	349	ASP	CA-C-N	5.17	125.25	119.87
2	F	349	ASP	C-N-CA	5.17	125.25	119.87
2	D	95	MET	O-C-N	-5.16	117.19	123.03
2	F	229	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	C	227	LYS	CA-C-O	-5.15	115.07	120.63
2	F	257	ASN	OD1-CG-ND2	5.15	127.75	122.60
1	A	330	GLN	CA-C-O	5.14	125.98	120.32
1	A	213	VAL	N-CA-C	-5.14	105.32	110.30
2	E	265	GLY	O-C-N	5.14	127.11	122.18
1	A	342	VAL	CA-C-O	5.13	126.02	120.47
2	F	354	THR	CA-C-O	-5.13	115.53	121.49
1	A	116	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	304	ARG	NE-CZ-NH1	-5.11	116.39	121.50
2	D	93	ARG	NE-CZ-NH1	5.11	126.61	121.50
2	F	442	GLN	O-C-N	5.11	127.33	122.07
2	E	31	PRO	N-CA-CB	5.10	108.18	103.39
1	A	74	VAL	CB-CA-C	5.09	117.96	110.98
1	B	350	ILE	CA-C-O	-5.09	115.08	120.48
1	B	260	ASN	OD1-CG-ND2	5.09	127.69	122.60
2	D	85	PRO	N-CA-CB	5.08	107.70	103.17
1	B	287	ARG	CA-C-N	5.08	125.61	120.38
1	B	287	ARG	C-N-CA	5.08	125.61	120.38
1	C	270	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	326	VAL	CA-C-O	-5.08	114.73	120.67
1	B	158	PRO	N-CA-CB	5.08	108.58	103.25
1	A	425	THR	CA-C-O	-5.07	115.48	120.90
2	E	249	GLN	N-CA-C	5.07	116.64	110.41
2	F	229	ARG	N-CA-C	-5.07	105.85	112.23
2	D	80	ALA	N-CA-C	5.06	112.58	108.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	155	PHE	CA-CB-CG	5.06	118.86	113.80
2	F	236	GLY	CA-C-N	5.05	127.81	120.79
2	F	236	GLY	C-N-CA	5.05	127.81	120.79
1	B	338	ILE	N-CA-CB	5.05	114.39	110.45
1	A	337	TYR	CA-C-O	-5.05	115.70	121.00
2	E	139	VAL	N-CA-CB	5.04	119.55	111.23
2	F	141	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	148	THR	N-CA-C	-5.03	106.99	113.23
2	F	224	GLU	CA-C-N	5.03	123.33	119.66
2	F	224	GLU	C-N-CA	5.03	123.33	119.66
1	C	431	GLY	CA-C-O	-5.01	116.66	121.92
1	C	325	PRO	N-CA-CB	5.00	107.70	103.35

There are no chirality outliers.

There are no planarity outliers.

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	144	0
1	B	3656	0	3765	169	0
1	C	3748	0	3844	164	0
2	D	3539	0	3592	133	0
2	E	3530	0	3587	175	0
2	F	3530	0	3587	138	0
3	G	945	0	1019	42	0
4	A	31	0	12	2	0
4	B	31	0	12	2	0
4	C	31	0	12	6	0
4	F	31	0	12	1	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	B	6	0	8	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	27	0	12	2	0
8	E	5	0	0	1	0
9	A	24	0	0	2	0
9	B	26	0	0	6	0
9	C	14	0	0	0	0
9	D	15	0	0	0	0
9	E	13	0	0	3	0
9	F	17	0	0	3	0
9	G	2	0	0	0	0
All	All	22941	0	23276	908	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 20.

All (908) 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:B:351:PHE:HE2	1:B:353:GLU:HG2	1.26	1.01
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.43	1.00
2:F:12:ARG:HE	2:F:74:LYS:HE2	1.27	1.00
1:C:294:TYR:HB3	1:C:298:VAL:HG21	1.48	0.94
3:G:20:THR:HG23	3:G:232:MET:HE3	1.51	0.93
2:F:282:GLN:H	2:F:282:GLN:HE21	1.00	0.92
2:D:196:LEU:HG	2:D:200:MET:HE2	1.52	0.92
2:D:282:GLN:H	2:D:282:GLN:HE21	0.95	0.91
2:E:223:ASN:HD22	2:E:223:ASN:H	1.19	0.91
2:F:252:LEU:HD23	2:F:305:THR:HB	1.53	0.90
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.52	0.90
2:E:276:PRO:HD2	3:G:266:ILE:HD11	1.53	0.90
1:B:351:PHE:CE2	1:B:353:GLU:HG2	2.09	0.88
2:F:223:ASN:HD22	2:F:223:ASN:H	1.22	0.88
2:E:388:ILE:HG23	2:E:393:MET:HB2	1.56	0.88
2:F:228:ALA:O	2:F:232:VAL:HG22	1.75	0.87
2:F:164:VAL:HG13	2:F:420:VAL:HG12	1.54	0.87
2:E:167:MET:HE3	2:E:420:VAL:HG11	1.57	0.85
2:D:282:GLN:H	2:D:282:GLN:NE2	1.73	0.85
2:E:449:TYR:HB3	2:E:452:LEU:HD12	1.57	0.84
2:D:366:GLU:O	2:D:370:VAL:HG23	1.77	0.83
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.59	0.83
1:B:62:MET:HG3	1:B:95:VAL:HG21	1.59	0.82
2:F:282:GLN:H	2:F:282:GLN:NE2	1.77	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ILE:HD12	1:C:338:ILE:H	1.44	0.81
1:C:175:LYS:HE2	4:C:600:ATP:O1B	1.80	0.80
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.63	0.80
1:A:218:LYS:HD2	2:D:128:VAL:HG21	1.64	0.79
1:C:404:ALA:C	1:C:406:PHE:H	1.89	0.79
2:D:63:MET:HE1	2:D:231:ARG:HB2	1.63	0.78
1:C:99:VAL:HG13	1:C:253:MET:HA	1.64	0.78
2:E:419:GLN:HA	2:E:429:GLY:HA3	1.64	0.78
1:A:94:ILE:HG12	1:A:95:VAL:H	1.48	0.77
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.67	0.77
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.67	0.77
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.66	0.77
2:F:282:GLN:HE21	2:F:282:GLN:N	1.81	0.77
1:A:140:ILE:HD11	1:A:143:ARG:HH22	1.49	0.76
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.67	0.76
1:B:453:LEU:HD13	1:B:461:ILE:HD12	1.68	0.75
1:C:288:PRO:HG2	2:D:270:ALA:HB1	1.68	0.75
2:E:223:ASN:H	2:E:223:ASN:ND2	1.83	0.74
2:E:84:ILE:HG21	2:E:235:THR:HG23	1.69	0.74
2:E:280:GLY:HA2	3:G:262:LEU:HD21	1.69	0.73
1:A:44:LEU:O	1:A:47:VAL:HG22	1.87	0.73
2:F:16:VAL:C	2:F:17:ILE:HD12	2.13	0.73
2:F:92:GLY:HA2	2:F:206:ILE:HD12	1.71	0.73
2:F:12:ARG:NE	2:F:74:LYS:HE2	2.03	0.72
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.70	0.72
2:D:84:ILE:HB	2:D:85:PRO:HD2	1.70	0.72
1:B:497:LEU:HA	1:B:500:ILE:HD12	1.72	0.72
1:A:389:THR:HB	1:A:449:VAL:HG21	1.71	0.72
2:D:80:ALA:HB1	2:D:81:PRO:HD2	1.73	0.71
2:D:282:GLN:HE21	2:D:282:GLN:N	1.81	0.71
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.72	0.71
2:E:224:GLU:O	2:E:229:ARG:NH1	2.23	0.70
1:A:49:ALA:O	1:A:50:GLU:HB2	1.91	0.70
1:A:87:ILE:H	1:A:87:ILE:HD12	1.56	0.70
2:F:136:GLY:HA3	2:F:431:LEU:HD12	1.74	0.70
2:D:370:VAL:HG21	2:D:438:ILE:HG23	1.73	0.69
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.74	0.69
2:E:189:ARG:HG2	2:E:222:MET:HE3	1.74	0.69
2:E:282:GLN:H	2:E:282:GLN:NE2	1.91	0.69
1:B:185:ASN:HB2	1:B:435:PRO:HB2	1.75	0.69
1:C:347:ASP:HA	1:C:373:ARG:HD2	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:GLN:NE2	4:C:600:ATP:H2'	2.07	0.69
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.56	0.69
2:D:346:PRO:HG3	2:D:418:PHE:CZ	2.28	0.68
2:E:282:GLN:H	2:E:282:GLN:HE21	1.40	0.68
1:A:62:MET:HE2	1:A:64:LEU:HD21	1.76	0.68
1:C:295:PRO:O	1:C:298:VAL:HG23	1.93	0.68
2:F:359:ASP:HB3	2:F:362:ILE:HD12	1.74	0.68
1:C:52:MET:HE1	1:C:76:PHE:CE2	2.29	0.68
2:E:276:PRO:HD2	3:G:266:ILE:CD1	2.21	0.68
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.75	0.68
1:C:179:ALA:HB1	1:C:267:ILE:HG12	1.74	0.68
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.28	0.68
2:E:151:LYS:HE3	2:E:296:ILE:HB	1.76	0.67
1:B:303:SER:HB2	2:F:222:MET:HB2	1.77	0.67
1:C:472:VAL:HG23	1:C:480:LEU:HD11	1.77	0.67
3:G:2:THR:HG22	3:G:5:ASP:H	1.60	0.67
1:C:355:GLU:O	1:C:359:LYS:HG3	1.95	0.67
2:F:270:ALA:HA	9:F:2012:HOH:O	1.95	0.66
2:D:253:LEU:HD21	2:D:255:ILE:HD11	1.77	0.66
2:E:390:ILE:HG21	3:G:28:ALA:HB3	1.76	0.66
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.76	0.66
2:D:228:ALA:O	2:D:232:VAL:HG22	1.95	0.66
2:D:242:TYR:CE1	2:D:246:GLN:HG3	2.30	0.66
1:C:400:VAL:HG12	1:C:418:LEU:HD21	1.78	0.66
1:C:423:ARG:HD3	1:C:461:ILE:HD11	1.76	0.66
2:D:163:THR:HA	2:D:166:ILE:HG22	1.76	0.66
1:A:34:ILE:HD11	1:A:79:ASP:HB3	1.76	0.66
1:B:486:ASP:C	1:B:488:LYS:H	2.04	0.66
2:F:396:LEU:HD13	2:F:400:ASP:HB3	1.78	0.66
1:C:336:ALA:HB3	1:C:339:PRO:HG2	1.77	0.65
1:A:267:ILE:HG13	1:A:324:LEU:HB2	1.78	0.65
1:A:469:LEU:O	1:A:473:ILE:HG13	1.97	0.65
2:D:393:MET:HG3	2:D:396:LEU:HD12	1.78	0.65
1:A:202:ILE:HG12	1:A:230:ILE:HD12	1.77	0.65
2:F:252:LEU:CD2	2:F:305:THR:HB	2.25	0.65
2:F:388:ILE:HD12	2:F:393:MET:HG2	1.78	0.65
1:B:80:LYS:HD3	2:E:33:LEU:HD12	1.77	0.65
2:F:130:GLN:HB3	2:F:357:ILE:CD1	2.27	0.65
2:F:405:SER:O	2:F:409:LYS:HG3	1.96	0.65
2:E:223:ASN:HD22	2:E:223:ASN:N	1.94	0.64
1:A:362:ARG:HA	1:A:363:PRO:C	2.21	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:49:VAL:HA	2:E:60:THR:HG22	1.77	0.64
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.80	0.64
2:E:387:ILE:H	2:E:387:ILE:HD12	1.62	0.64
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.80	0.64
2:F:13:ILE:CD1	2:F:69:LEU:HD13	2.28	0.64
2:D:374:VAL:HG13	2:D:410:ILE:HG21	1.78	0.64
1:A:408:SER:O	1:A:409:ASP:HB2	1.98	0.64
1:C:404:ALA:C	1:C:406:PHE:N	2.56	0.64
2:E:200:MET:HB3	2:E:206:ILE:HG13	1.79	0.64
1:B:185:ASN:HB2	1:B:435:PRO:CB	2.28	0.64
1:C:292:GLU:O	1:C:293:ALA:HB3	1.98	0.63
2:D:96:ASN:HB2	2:D:100:GLU:O	1.99	0.63
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.81	0.63
2:E:32:ILE:O	2:E:33:LEU:HB2	1.97	0.63
1:B:78:ASN:OD1	1:B:80:LYS:HG2	1.99	0.63
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.29	0.63
1:A:196:LYS:H	1:A:196:LYS:HD2	1.64	0.62
2:E:48:GLU:OE2	2:E:231:ARG:NH2	2.30	0.62
1:B:486:ASP:C	1:B:488:LYS:N	2.56	0.62
1:A:432:GLN:OE1	4:A:600:ATP:H2'	1.99	0.62
1:A:440:GLU:HB3	1:A:469:LEU:HD11	1.81	0.62
1:B:171:ARG:HH22	2:E:356:ARG:HH21	1.47	0.62
2:E:280:GLY:HA2	3:G:262:LEU:CD2	2.29	0.62
2:F:406:ARG:HH21	2:F:447:GLY:HA3	1.65	0.62
1:B:151:LYS:HG3	1:B:430:GLN:OE1	1.99	0.62
2:F:287:THR:O	2:F:291:THR:HG23	2.00	0.62
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.80	0.62
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.81	0.62
1:C:127:ARG:HH21	1:C:131:LEU:HD12	1.64	0.62
2:E:404:VAL:O	2:E:408:ARG:HG3	2.00	0.62
1:A:188:ARG:NH2	1:A:436:MET:HA	2.14	0.61
2:D:29:LEU:HD12	2:D:30:PRO:HD2	1.82	0.61
1:A:146:MET:HE3	1:A:146:MET:O	2.00	0.61
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.83	0.61
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.31	0.61
1:C:215:GLN:HG3	2:F:356:ARG:HH12	1.64	0.61
1:B:158:PRO:O	1:B:375:GLY:HA3	2.00	0.61
1:C:362:ARG:HA	1:C:363:PRO:C	2.25	0.61
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.31	0.61
1:C:44:LEU:O	1:C:47:VAL:HG22	2.01	0.61
1:C:107:VAL:HB	1:C:116:ASP:HB3	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:10:LEU:HD21	3:G:246:LEU:HB2	1.83	0.61
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.83	0.60
2:F:164:VAL:HG13	2:F:420:VAL:CG1	2.27	0.60
1:A:390:MET:HE3	1:A:424:LEU:HD22	1.81	0.60
2:E:170:ILE:HG12	2:E:181:SER:CB	2.32	0.60
2:F:443:GLN:HE21	2:F:449:TYR:HE2	1.47	0.60
2:E:96:ASN:HD22	2:E:100:GLU:HB2	1.66	0.60
1:B:134:PRO:HD3	9:B:2012:HOH:O	2.01	0.60
2:E:66:THR:HB	2:E:69:LEU:HD12	1.83	0.60
2:F:245:ASP:C	2:F:247:GLU:H	2.10	0.60
1:B:65:ASN:ND2	2:F:17:ILE:HG23	2.16	0.60
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.65	0.60
1:B:420:ARG:HH21	1:B:451:GLY:HA2	1.66	0.60
1:B:468:PHE:CE1	1:B:501:VAL:HG12	2.36	0.59
2:F:13:ILE:HD13	2:F:69:LEU:HD13	1.82	0.59
2:E:170:ILE:HD13	2:E:215:VAL:CG2	2.31	0.59
1:B:453:LEU:HD13	1:B:461:ILE:HG23	1.83	0.59
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.84	0.59
1:B:419:SER:O	1:B:423:ARG:HG2	2.01	0.59
1:C:27:GLU:OE2	1:C:46:ASN:ND2	2.34	0.59
2:D:408:ARG:NH1	2:D:454:GLU:OE1	2.35	0.59
1:B:246:ALA:HB3	1:B:247:PRO:HD3	1.83	0.59
1:C:97:VAL:O	1:C:99:VAL:HG23	2.02	0.59
1:B:44:LEU:O	1:B:47:VAL:HG22	2.02	0.59
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.84	0.59
3:G:81:ILE:HG22	3:G:82:HIS:HD2	1.68	0.59
1:B:350:ILE:CG2	1:B:365:ILE:HG12	2.33	0.59
1:A:204:VAL:HG12	1:A:206:ILE:HD11	1.85	0.58
1:C:295:PRO:HD2	1:C:298:VAL:CG2	2.33	0.58
1:B:452:TYR:OH	1:B:498:LYS:HG3	2.03	0.58
2:F:151:LYS:HD3	2:F:328:HIS:O	2.03	0.58
1:B:304:ARG:NH2	6:B:701:GOL:O2	2.37	0.58
1:C:468:PHE:CE1	1:C:501:VAL:HG12	2.39	0.58
2:E:126:MET:HE1	2:E:297:THR:HG21	1.85	0.58
2:D:9:THR:HG22	2:D:27:GLU:OE1	2.03	0.58
3:G:13:ILE:HD13	3:G:242:MET:SD	2.43	0.58
1:B:381:ARG:O	1:B:385:GLN:HG3	2.03	0.58
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.84	0.58
2:F:89:GLU:CD	2:F:89:GLU:H	2.10	0.58
2:F:275:ILE:O	2:F:283:PRO:HG3	2.03	0.58
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:MET:HE1	1:C:76:PHE:HE2	1.68	0.58
2:D:419:GLN:O	2:D:422:GLU:HG3	2.03	0.58
1:A:313:ASN:OD1	1:A:316:PHE:HD1	1.87	0.58
2:D:101:PRO:HD3	2:D:108:ILE:HD12	1.86	0.58
2:D:130:GLN:HE22	2:D:356:ARG:HG2	1.68	0.58
2:D:143:LEU:CD1	2:D:350:PRO:HB3	2.34	0.57
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.86	0.57
1:C:23:VAL:HG12	1:C:23:VAL:O	2.04	0.57
1:C:335:SER:O	2:D:314:ALA:HB1	2.04	0.57
2:D:345:TYR:HA	2:D:346:PRO:C	2.28	0.57
2:E:231:ARG:O	2:E:234:LEU:HB2	2.04	0.57
2:F:94:ILE:HG12	2:F:217:LEU:HD12	1.85	0.57
2:E:352:ASP:O	2:E:354:THR:HG23	2.04	0.57
2:E:422:GLU:HG2	2:E:427:HIS:O	2.03	0.57
2:F:422:GLU:HG2	2:F:427:HIS:O	2.04	0.57
1:B:251:CYS:HB2	1:B:268:TYR:OH	2.04	0.57
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.39	0.57
1:A:99:VAL:HG22	1:A:253:MET:HA	1.87	0.57
2:D:49:VAL:HA	2:D:60:THR:HG22	1.86	0.57
3:G:210:ALA:O	3:G:211:ASN:C	2.47	0.57
1:A:140:ILE:CD1	1:A:143:ARG:HH22	2.16	0.57
2:F:166:ILE:O	2:F:170:ILE:HG13	2.05	0.57
1:C:26:GLU:HA	1:C:45:ARG:HB2	1.86	0.57
2:E:254:PHE:HA	2:E:307:VAL:O	2.04	0.57
1:A:99:VAL:CG2	1:A:253:MET:HA	2.35	0.57
1:A:389:THR:HG22	1:A:393:GLU:OE2	2.05	0.57
2:D:417:PRO:CA	2:D:459:MET:HE1	2.35	0.57
2:F:174:ALA:O	2:F:177:HIS:HB3	2.04	0.57
1:A:497:LEU:O	1:A:501:VAL:HG22	2.04	0.56
1:A:151:LYS:HE2	1:A:427:LEU:O	2.05	0.56
1:C:327:ILE:HD11	1:C:342:VAL:HG21	1.87	0.56
2:F:446:ALA:HB3	2:F:448:GLU:HG3	1.87	0.56
1:A:127:ARG:HD3	1:A:252:SER:HB3	1.87	0.56
1:B:64:LEU:HG	1:B:65:ASN:ND2	2.20	0.56
2:D:292:MET:HE2	2:D:293:GLN:HG2	1.87	0.56
2:F:130:GLN:HB3	2:F:357:ILE:HD12	1.86	0.56
2:F:223:ASN:HD22	2:F:223:ASN:N	1.97	0.56
1:B:286:ARG:HA	2:E:275:ILE:HD12	1.86	0.56
1:B:420:ARG:HH21	1:B:451:GLY:CA	2.19	0.56
1:B:496:LYS:HG2	1:B:500:ILE:HD11	1.88	0.56
1:C:128:ARG:O	1:C:252:SER:OG	2.24	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:38:LEU:HD11	3:G:42:ARG:NH2	2.21	0.56
1:B:187:LYS:NZ	1:B:224:ASP:HB3	2.20	0.56
1:B:383:MET:SD	1:B:387:ALA:HB2	2.45	0.56
1:C:174:GLY:HA2	4:C:600:ATP:PA	2.45	0.56
1:C:295:PRO:HD2	1:C:298:VAL:HG22	1.88	0.56
2:D:360:PRO:HD3	2:D:368:TYR:CD1	2.40	0.56
1:C:343:ILE:HG22	2:D:158:ALA:HB1	1.87	0.56
1:C:414:THR:O	1:C:418:LEU:HG	2.06	0.56
1:C:452:TYR:OH	1:C:498:LYS:HD2	2.06	0.56
2:D:430:LYS:HD2	2:D:465:GLU:OE2	2.05	0.56
1:B:26:GLU:HB3	1:B:46:ASN:ND2	2.20	0.56
2:D:292:MET:CE	2:D:293:GLN:HG2	2.36	0.56
2:F:345:TYR:HA	2:F:346:PRO:C	2.30	0.56
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.71	0.56
2:F:84:ILE:HD13	2:F:235:THR:HG23	1.88	0.56
2:D:63:MET:CE	2:D:97:VAL:HG11	2.37	0.55
1:B:209:LYS:HB3	2:E:294:GLU:OE2	2.06	0.55
1:C:338:ILE:O	1:C:339:PRO:C	2.47	0.55
1:A:204:VAL:CG1	1:A:206:ILE:HD11	2.36	0.55
2:D:279:VAL:HG12	2:D:279:VAL:O	2.06	0.55
1:B:288:PRO:HB3	2:F:276:PRO:HG3	1.89	0.55
2:F:415:SER:HB2	2:F:459:MET:HE2	1.89	0.55
1:A:36:ASP:O	1:A:284:LEU:HD13	2.07	0.55
1:B:366:ASN:ND2	1:B:369:LEU:HD12	2.21	0.55
1:B:468:PHE:O	1:B:472:VAL:HG22	2.07	0.55
1:B:171:ARG:NH1	1:B:171:ARG:HB2	2.22	0.55
1:C:291:ARG:HD3	1:C:337:TYR:CE1	2.41	0.55
1:B:165:GLU:O	1:B:325:PRO:HD2	2.06	0.55
1:C:225:ALA:HA	1:C:228:TYR:CE2	2.42	0.54
2:D:324:THR:HG22	2:D:324:THR:O	2.07	0.54
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.88	0.54
1:A:188:ARG:NH2	1:A:436:MET:C	2.66	0.54
1:B:188:ARG:HG2	1:B:188:ARG:HH11	1.72	0.54
3:G:6:ILE:HG21	3:G:250:PHE:HB2	1.90	0.54
1:C:105:GLY:HA2	1:C:226:MET:O	2.07	0.54
1:C:170:ASP:O	1:C:175:LYS:NZ	2.40	0.54
1:B:338:ILE:HB	1:B:339:PRO:HD3	1.89	0.54
2:D:16:VAL:HG13	2:D:21:VAL:HG22	1.89	0.54
2:E:96:ASN:OD1	2:E:97:VAL:HG23	2.08	0.54
1:C:443:ALA:O	1:C:446:TYR:HB3	2.07	0.54
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HG13	2:E:194:ASN:HB2	1.89	0.54
1:A:188:ARG:HH22	1:A:436:MET:HA	1.73	0.54
1:B:171:ARG:HB2	1:B:171:ARG:HH11	1.73	0.54
2:D:388:ILE:HG21	2:D:396:LEU:HD11	1.90	0.54
1:B:146:MET:HG3	1:B:322:THR:HG21	1.89	0.53
1:B:210:ARG:O	1:B:211:SER:C	2.51	0.53
1:B:410:LEU:O	1:B:411:ASP:HB3	2.08	0.53
1:C:146:MET:HE3	1:C:146:MET:O	2.07	0.53
2:D:363:VAL:HB	2:D:367:HIS:ND1	2.23	0.53
2:E:264:ALA:O	2:E:268:VAL:HG23	2.08	0.53
2:F:393:MET:SD	2:F:404:VAL:HG11	2.48	0.53
1:A:157:VAL:N	1:A:158:PRO:CD	2.71	0.53
1:A:440:GLU:O	1:A:444:VAL:HG13	2.07	0.53
1:A:486:ASP:OD2	1:A:490:SER:HB3	2.08	0.53
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.91	0.53
2:F:241:GLU:CD	2:F:295:ARG:HH21	2.16	0.53
1:A:48:GLN:HG2	2:E:70:VAL:HG22	1.91	0.53
2:E:390:ILE:HG21	3:G:28:ALA:CB	2.38	0.53
2:E:170:ILE:HD13	2:E:215:VAL:HG21	1.89	0.53
1:B:347:ASP:C	1:B:373:ARG:HG3	2.34	0.53
2:F:319:ASP:O	2:F:320:PRO:C	2.52	0.53
2:E:357:ILE:HB	2:E:362:ILE:HG21	1.90	0.53
2:E:454:GLU:O	2:E:456:ALA:N	2.42	0.53
1:C:55:PHE:O	1:C:56:SER:C	2.51	0.53
2:D:234:LEU:CD2	2:D:292:MET:HG3	2.39	0.53
2:F:223:ASN:H	2:F:223:ASN:ND2	2.00	0.53
2:D:277:SER:OG	2:D:278:ALA:N	2.41	0.53
2:D:410:ILE:HD11	2:D:445:LEU:HD23	1.91	0.53
1:B:65:ASN:HD22	2:F:17:ILE:HG23	1.74	0.53
1:B:190:ASN:HA	1:B:198:LYS:HG2	1.90	0.53
2:E:367:HIS:HA	2:E:438:ILE:HD12	1.91	0.52
2:F:84:ILE:O	2:F:84:ILE:HG13	2.08	0.52
1:A:188:ARG:HH21	1:A:437:ALA:N	2.07	0.52
1:B:102:GLU:HG3	1:B:122:GLY:C	2.33	0.52
1:B:174:GLY:HA2	4:B:600:ATP:PA	2.50	0.52
2:E:282:GLN:HE21	2:E:282:GLN:N	2.07	0.52
2:F:161:GLY:HA3	9:F:2007:HOH:O	2.09	0.52
2:D:151:LYS:HE2	2:D:328:HIS:O	2.10	0.52
2:F:111:LYS:HB2	2:F:112:GLN:OE1	2.10	0.52
1:B:248:TYR:CG	6:B:701:GOL:H12	2.45	0.52
1:B:300:TYR:HA	1:B:303:SER:HG	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:VAL:O	1:C:308:ARG:NH1	2.42	0.52
3:G:20:THR:HG22	3:G:236:SER:HB3	1.92	0.52
1:A:94:ILE:HG21	1:A:128:ARG:NH1	2.24	0.52
1:A:419:SER:O	1:A:423:ARG:HD3	2.10	0.52
1:B:327:ILE:HD11	1:B:342:VAL:HG21	1.92	0.52
1:C:152:ALA:CB	1:C:365:ILE:HD12	2.39	0.52
2:D:93:ARG:NH2	2:D:106:GLY:O	2.26	0.52
1:C:75:VAL:HG21	1:C:79:ASP:HB3	1.91	0.52
2:D:408:ARG:HD3	2:D:454:GLU:OE2	2.09	0.52
1:A:180:ILE:O	1:A:181:ASP:C	2.53	0.51
1:A:376:SER:O	1:A:377:ALA:C	2.52	0.51
1:C:44:LEU:O	2:D:71:ARG:NH2	2.43	0.51
1:B:157:VAL:N	1:B:158:PRO:CD	2.73	0.51
1:C:404:ALA:O	1:C:406:PHE:N	2.43	0.51
2:E:84:ILE:HD13	2:E:235:THR:HG23	1.92	0.51
2:E:415:SER:HB2	2:E:459:MET:SD	2.51	0.51
1:A:503:ASN:O	1:A:506:ALA:HB3	2.10	0.51
1:B:55:PHE:O	1:B:56:SER:C	2.53	0.51
2:D:161:GLY:O	2:D:162:LYS:C	2.51	0.51
2:D:186:VAL:HG12	2:D:260:ARG:HB2	1.92	0.51
1:A:137:ILE:N	1:A:138:PRO:CD	2.73	0.51
1:A:339:PRO:O	1:A:343:ILE:HG13	2.10	0.51
1:C:30:ARG:HG2	1:C:30:ARG:HH11	1.76	0.51
1:C:48:GLN:HG2	2:D:70:VAL:CG2	2.39	0.51
1:C:52:MET:HE1	1:C:76:PHE:CD2	2.45	0.51
2:D:9:THR:HG21	2:D:28:GLY:H	1.74	0.51
2:E:258:ILE:CG2	2:E:310:ILE:HG12	2.40	0.51
1:C:418:LEU:O	1:C:422:VAL:HG23	2.11	0.51
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.92	0.51
1:A:278:TYR:HA	1:A:281:MET:HE2	1.92	0.51
1:C:303:SER:HB2	2:D:222:MET:HB3	1.92	0.51
2:D:145:PRO:HB2	2:D:357:ILE:HD11	1.91	0.51
2:D:201:ILE:CD1	2:D:208:LEU:HD11	2.41	0.51
2:F:357:ILE:O	2:F:359:ASP:N	2.43	0.51
1:A:107:VAL:HG13	1:A:231:VAL:HG12	1.92	0.51
1:C:291:ARG:HD3	1:C:337:TYR:CD1	2.45	0.51
2:D:252:LEU:HD23	2:D:305:THR:HB	1.92	0.51
2:F:247:GLU:HG2	2:F:249:GLN:HG2	1.91	0.51
1:B:62:MET:HG3	1:B:95:VAL:CG2	2.35	0.51
1:B:468:PHE:CZ	1:B:501:VAL:HG12	2.45	0.51
1:C:373:ARG:HA	7:D:600:ADP:O3'	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:LEU:HD11	1:C:497:LEU:HG	1.92	0.51
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.38	0.51
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.92	0.51
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.92	0.51
1:A:439:GLU:CD	1:A:439:GLU:H	2.19	0.51
2:E:405:SER:O	2:E:409:LYS:HG3	2.10	0.51
2:E:434:LEU:O	2:E:438:ILE:HG12	2.11	0.51
1:A:403:PHE:CD1	3:G:22:SER:HB2	2.46	0.51
1:A:457:GLU:HB3	1:A:460:LYS:HE3	1.92	0.51
1:B:52:MET:HE2	1:B:95:VAL:HG13	1.93	0.50
1:B:175:LYS:NZ	9:B:2006:HOH:O	2.43	0.50
1:B:280:GLN:CD	2:E:284:THR:HG22	2.36	0.50
1:C:74:VAL:HG13	1:C:241:PRO:CG	2.41	0.50
2:F:357:ILE:HG23	2:F:362:ILE:HG21	1.93	0.50
1:A:411:ASP:OD2	1:A:414:THR:HG23	2.12	0.50
2:E:321:ALA:N	2:E:322:PRO:HD2	2.27	0.50
3:G:39:LYS:N	3:G:40:PRO:HD2	2.26	0.50
1:B:157:VAL:O	1:B:159:ILE:HD13	2.11	0.50
1:C:362:ARG:HD3	4:C:600:ATP:C2	2.46	0.50
2:F:406:ARG:HH21	2:F:447:GLY:CA	2.24	0.50
1:C:174:GLY:HA2	4:C:600:ATP:O5'	2.12	0.50
2:D:165:LEU:O	2:D:169:LEU:HG	2.11	0.50
2:D:139:VAL:HG12	2:D:143:LEU:HD12	1.93	0.50
3:G:38:LEU:O	3:G:42:ARG:HG3	2.10	0.50
1:C:382:ALA:HA	1:C:385:GLN:OE1	2.12	0.50
2:D:319:ASP:O	2:D:320:PRO:C	2.54	0.50
2:E:275:ILE:HG23	3:G:266:ILE:HD13	1.93	0.50
2:F:63:MET:HE1	2:F:231:ARG:CB	2.42	0.50
2:F:346:PRO:HG3	2:F:418:PHE:CZ	2.46	0.50
1:A:400:VAL:HG12	1:A:418:LEU:HD21	1.93	0.50
1:B:339:PRO:O	1:B:343:ILE:HG13	2.11	0.50
1:B:423:ARG:O	1:B:426:GLU:N	2.44	0.50
2:D:89:GLU:HG2	2:D:110:THR:CG2	2.41	0.50
2:E:31:PRO:HD2	2:E:34:ASN:ND2	2.27	0.50
2:E:185:GLY:HA3	2:E:188:GLU:HG2	1.93	0.50
1:C:434:SER:N	1:C:435:PRO:HD3	2.26	0.50
2:E:89:GLU:OE2	2:E:110:THR:HG22	2.11	0.50
1:C:110:ALA:HB2	1:C:246:ALA:HB2	1.94	0.49
1:C:127:ARG:NH2	1:C:131:LEU:HD12	2.26	0.49
2:F:164:VAL:HG23	4:F:600:ATP:O1A	2.13	0.49
1:B:479:LEU:CD1	1:B:497:LEU:HD13	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:393:MET:HG3	2:E:396:LEU:HD11	1.94	0.49
1:B:141:SER:O	1:B:143:ARG:HD2	2.13	0.49
1:B:167:ILE:HG22	1:B:175:LYS:HG2	1.95	0.49
2:D:9:THR:HG22	2:D:27:GLU:HB2	1.95	0.49
2:E:203:SER:HB2	2:E:420:VAL:HG13	1.95	0.49
1:A:151:LYS:NZ	1:A:430:GLN:HB2	2.26	0.49
1:B:106:ARG:NH1	1:B:121:ILE:HD13	2.27	0.49
1:B:400:VAL:HG12	1:B:418:LEU:HD21	1.93	0.49
1:C:438:ILE:O	1:C:442:VAL:HG23	2.12	0.49
2:E:116:ILE:HA	2:E:238:THR:OG1	2.12	0.49
1:C:292:GLU:O	1:C:293:ALA:CB	2.61	0.49
2:E:149:GLY:HA2	2:E:304:ILE:O	2.12	0.49
2:F:134:VAL:HA	2:F:141:ASP:OD1	2.13	0.49
2:F:346:PRO:HG3	2:F:418:PHE:HZ	1.78	0.49
1:B:361:ILE:HD12	1:B:429:LYS:HE2	1.94	0.49
2:D:314:ALA:O	2:D:315:ASP:HB2	2.11	0.49
2:E:360:PRO:HG3	2:E:368:TYR:CD2	2.48	0.49
3:G:28:ALA:HA	3:G:229:MET:SD	2.53	0.49
1:B:94:ILE:O	1:B:95:VAL:C	2.56	0.49
1:B:151:LYS:NZ	1:B:430:GLN:HB2	2.28	0.49
1:B:299:PHE:HB3	9:B:2017:HOH:O	2.11	0.49
2:E:399:GLU:O	2:E:403:THR:HG23	2.12	0.49
2:D:162:LYS:HE3	2:D:311:TYR:HA	1.94	0.49
2:F:221:GLN:NE2	2:F:221:GLN:HA	2.27	0.49
2:F:367:HIS:HA	2:F:438:ILE:HD12	1.93	0.49
1:C:168:ILE:O	1:C:351:PHE:HA	2.12	0.49
2:E:25:PHE:HB2	2:E:29:LEU:HD12	1.94	0.49
2:E:151:LYS:HB2	2:E:328:HIS:O	2.13	0.49
2:E:174:ALA:HB3	2:E:214:LYS:HD3	1.94	0.49
2:E:384:LEU:O	2:E:385:GLN:C	2.55	0.49
2:F:51:GLN:HG2	2:F:59:ARG:HB3	1.95	0.49
2:F:95:MET:HE3	2:F:108:ILE:HD13	1.94	0.49
3:G:81:ILE:HG22	3:G:82:HIS:N	2.28	0.49
1:B:98:PRO:O	1:B:99:VAL:HG23	2.13	0.49
1:C:240:ALA:N	1:C:241:PRO:CD	2.75	0.49
1:C:297:ASP:HA	2:D:267:GLU:HG2	1.94	0.49
1:B:59:LEU:HD12	9:B:2001:HOH:O	2.12	0.48
2:E:151:LYS:HG2	2:E:293:GLN:OE1	2.13	0.48
2:E:257:ASN:HB2	2:E:309:ALA:O	2.13	0.48
2:F:188:GLU:O	2:F:221:GLN:HB3	2.13	0.48
2:F:324:THR:O	2:F:324:THR:HG22	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:NH2	1:A:437:ALA:N	2.60	0.48
1:B:486:ASP:O	1:B:488:LYS:N	2.46	0.48
2:D:417:PRO:HG2	2:D:430:LYS:H	1.78	0.48
2:D:439:LYS:O	2:D:443:GLN:HG3	2.11	0.48
2:D:474:ALA:O	2:D:475:GLU:HB2	2.14	0.48
1:C:100:GLY:HA2	1:C:256:TYR:CE2	2.48	0.48
1:C:213:VAL:O	1:C:216:LEU:HB3	2.13	0.48
2:D:89:GLU:CD	2:D:89:GLU:H	2.20	0.48
2:D:346:PRO:HG3	2:D:418:PHE:HZ	1.74	0.48
2:E:196:LEU:HD23	2:E:219:TYR:OH	2.13	0.48
2:E:221:GLN:N	2:E:224:GLU:OE2	2.44	0.48
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.36	0.48
1:A:87:ILE:HD12	1:A:87:ILE:N	2.27	0.48
1:A:180:ILE:O	1:A:184:ILE:HG12	2.12	0.48
1:A:213:VAL:O	1:A:216:LEU:HB3	2.14	0.48
1:C:211:SER:HB3	2:F:126:MET:HE2	1.96	0.48
2:F:116:ILE:HA	2:F:238:THR:OG1	2.13	0.48
1:B:127:ARG:HE	1:B:131:LEU:HD12	1.78	0.48
2:D:285:LEU:C	2:D:285:LEU:HD23	2.39	0.48
2:E:120:ALA:O	2:E:121:PRO:C	2.56	0.48
1:B:211:SER:N	2:E:126:MET:HE2	2.29	0.48
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.48	0.48
1:C:176:THR:OG1	1:C:269:ASP:OD2	2.32	0.48
1:C:323:ALA:O	1:C:324:LEU:HD23	2.14	0.48
1:A:184:ILE:HB	1:A:435:PRO:HG3	1.95	0.48
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.94	0.48
1:C:76:PHE:HB3	1:C:242:LEU:HD21	1.96	0.48
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.95	0.48
2:F:89:GLU:OE2	2:F:110:THR:HG22	2.14	0.48
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.79	0.48
1:A:484:ARG:O	1:A:485:THR:C	2.57	0.48
3:G:222:THR:O	3:G:226:SER:OG	2.31	0.48
1:A:151:LYS:NZ	1:A:430:GLN:OE1	2.47	0.48
1:A:185:ASN:OD1	1:A:188:ARG:NH1	2.46	0.48
1:A:286:ARG:NH2	3:G:272:LEU:HD13	2.29	0.48
1:A:479:LEU:O	1:A:479:LEU:HD22	2.14	0.48
1:C:432:GLN:O	1:C:433:TYR:HB2	2.14	0.48
1:C:476:HIS:CD2	1:C:500:ILE:HD11	2.48	0.48
2:F:366:GLU:O	2:F:370:VAL:HG23	2.13	0.48
1:A:175:LYS:HE3	4:A:600:ATP:O1B	2.14	0.47
1:A:240:ALA:N	1:A:241:PRO:CD	2.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LYS:HG3	1:B:81:LEU:N	2.29	0.47
1:B:133:ALA:HB1	1:B:134:PRO:HD2	1.96	0.47
1:B:146:MET:SD	1:B:146:MET:C	2.97	0.47
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.49	0.47
1:B:441:GLN:O	1:B:445:ILE:HG12	2.14	0.47
1:C:137:ILE:HG21	2:D:104:GLU:OE1	2.14	0.47
1:A:180:ILE:HD11	1:A:216:LEU:CD2	2.44	0.47
1:B:361:ILE:CD1	1:B:429:LYS:HE2	2.44	0.47
1:A:468:PHE:O	1:A:472:VAL:HG13	2.14	0.47
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.44	0.47
1:B:201:CYS:O	1:B:229:THR:HA	2.14	0.47
1:C:211:SER:CB	2:F:126:MET:HE2	2.44	0.47
2:E:449:TYR:CE2	2:E:463:ILE:HG12	2.49	0.47
1:A:97:VAL:HG11	1:A:249:SER:HB3	1.97	0.47
1:A:144:GLU:HB2	1:A:161:ARG:HG3	1.96	0.47
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.43	0.47
1:B:388:GLY:O	1:B:392:LEU:HG	2.13	0.47
2:E:89:GLU:HG3	2:E:109:LYS:O	2.15	0.47
1:C:185:ASN:OD1	1:C:435:PRO:HB2	2.15	0.47
2:E:462:PRO:HG2	2:E:465:GLU:HG3	1.96	0.47
1:A:156:LEU:HD13	1:A:367:VAL:HG11	1.96	0.47
1:A:297:ASP:HA	9:E:2009:HOH:O	2.13	0.47
2:E:10:THR:HG23	2:E:76:LEU:HD23	1.97	0.47
2:E:256:ASP:HA	2:E:257:ASN:HA	1.58	0.47
1:A:117:GLY:C	1:A:119:GLY:H	2.23	0.47
1:B:210:ARG:NH1	2:E:121:PRO:O	2.45	0.47
2:D:92:GLY:HA2	2:D:206:ILE:HG12	1.96	0.47
2:D:163:THR:O	2:D:164:VAL:C	2.55	0.47
2:D:339:ILE:O	2:D:340:ALA:C	2.57	0.47
2:D:411:GLN:O	2:D:414:LEU:HB2	2.13	0.47
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.96	0.47
2:E:455:GLN:O	2:E:469:LYS:HD3	2.15	0.47
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.44	0.47
1:A:286:ARG:HG2	1:A:286:ARG:HH11	1.79	0.47
1:B:141:SER:OG	1:B:143:ARG:NH1	2.47	0.47
1:B:194:ASP:C	1:B:196:LYS:H	2.22	0.47
1:C:40:ARG:NH1	1:C:70:ASN:OD1	2.48	0.47
1:C:130:GLY:O	1:C:131:LEU:C	2.57	0.47
1:C:186:GLN:HA	1:C:189:PHE:CE2	2.50	0.47
1:C:360:GLY:HA2	1:C:362:ARG:NH1	2.30	0.47
2:D:198:HIS:O	2:D:202:GLU:HG2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:417:PRO:HA	2:D:459:MET:HE1	1.97	0.47
2:E:139:VAL:HG13	2:E:414:LEU:HB3	1.97	0.47
3:G:237:LYS:O	3:G:241:GLU:HG3	2.15	0.47
2:D:258:ILE:HD11	2:D:292:MET:SD	2.55	0.47
2:D:432:VAL:HA	2:D:433:PRO:HD3	1.83	0.47
2:E:105:ARG:NH1	2:E:208:LEU:HD23	2.30	0.47
2:F:243:PHE:HB2	2:F:251:VAL:CG2	2.44	0.47
3:G:32:ALA:O	3:G:36:ARG:HG3	2.15	0.47
3:G:209:LEU:O	3:G:210:ALA:C	2.58	0.47
1:A:159:ILE:CD1	1:A:165:GLU:HG2	2.45	0.46
1:C:166:LEU:HD13	1:C:342:VAL:CG1	2.46	0.46
2:D:412:ARG:C	2:D:414:LEU:N	2.73	0.46
1:A:397:TYR:CG	1:A:421:GLY:HA3	2.50	0.46
1:B:32:LEU:HG	1:B:42:HIS:HB2	1.96	0.46
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.97	0.46
2:E:259:PHE:HE1	2:E:313:PRO:HG3	1.78	0.46
1:A:103:LEU:HD13	1:A:253:MET:SD	2.56	0.46
1:B:66:LEU:O	2:F:15:ALA:HA	2.15	0.46
1:B:481:GLY:HA2	1:B:484:ARG:CZ	2.45	0.46
2:E:374:VAL:HG13	2:E:410:ILE:HG21	1.96	0.46
2:F:118:ALA:O	2:F:295:ARG:HD2	2.15	0.46
2:E:105:ARG:HD3	9:E:2006:HOH:O	2.15	0.46
2:E:258:ILE:HG22	2:E:310:ILE:HG12	1.96	0.46
1:B:186:GLN:HG3	1:B:199:LEU:HD23	1.96	0.46
1:C:446:TYR:O	1:C:447:ALA:C	2.59	0.46
2:F:95:MET:HG2	2:F:218:VAL:HG22	1.96	0.46
1:A:156:LEU:CD2	1:A:391:LYS:HB2	2.45	0.46
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.98	0.46
2:D:181:SER:O	2:D:215:VAL:HA	2.15	0.46
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.81	0.46
1:A:140:ILE:CG2	1:A:313:ASN:HA	2.45	0.46
1:A:188:ARG:NH2	1:A:436:MET:CA	2.79	0.46
1:A:204:VAL:HG12	1:A:206:ILE:CD1	2.46	0.46
1:B:54:GLU:HG3	1:B:91:THR:HG22	1.97	0.46
1:C:162:GLY:HA2	1:C:321:LEU:O	2.16	0.46
1:A:166:LEU:HD21	1:A:168:ILE:HB	1.97	0.46
1:A:479:LEU:O	1:A:483:ILE:HG13	2.16	0.46
2:D:9:THR:CG2	2:D:27:GLU:HB2	2.45	0.46
1:B:179:ALA:O	1:B:182:THR:HB	2.16	0.46
1:B:362:ARG:HA	1:B:363:PRO:C	2.40	0.46
1:B:423:ARG:HD2	1:B:461:ILE:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:LYS:HG2	1:C:489:ILE:N	2.31	0.46
2:E:422:GLU:OE1	2:E:428:LEU:HA	2.16	0.46
1:B:151:LYS:HE2	1:B:427:LEU:O	2.15	0.46
1:B:286:ARG:HA	2:E:275:ILE:CD1	2.45	0.46
1:B:300:TYR:HA	1:B:303:SER:OG	2.16	0.46
1:C:45:ARG:NH2	1:C:68:PRO:O	2.49	0.46
1:C:210:ARG:NH1	2:F:121:PRO:O	2.48	0.46
2:E:419:GLN:CA	2:E:429:GLY:HA3	2.42	0.46
2:F:53:LEU:HD21	2:F:59:ARG:HB2	1.97	0.46
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.98	0.46
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.97	0.46
1:A:138:PRO:HB3	1:A:316:PHE:CZ	2.51	0.45
1:A:156:LEU:HD13	1:A:367:VAL:CG1	2.46	0.45
1:A:338:ILE:N	1:A:339:PRO:CD	2.78	0.45
1:C:338:ILE:HB	1:C:339:PRO:CD	2.46	0.45
3:G:5:ASP:O	3:G:6:ILE:C	2.60	0.45
3:G:228:ARG:O	3:G:232:MET:HG2	2.16	0.45
1:B:278:TYR:OH	1:B:297:ASP:OD2	2.30	0.45
1:C:168:ILE:HG23	1:C:351:PHE:HD1	1.80	0.45
2:D:170:ILE:O	2:D:174:ALA:HB3	2.16	0.45
2:E:246:GLN:HA	2:E:246:GLN:HE21	1.82	0.45
2:E:408:ARG:O	2:E:412:ARG:HG3	2.16	0.45
1:A:94:ILE:HG12	1:A:95:VAL:N	2.25	0.45
1:B:240:ALA:HB3	1:B:241:PRO:HD3	1.97	0.45
2:D:452:LEU:HD22	2:D:470:ALA:CB	2.47	0.45
2:E:201:ILE:HD13	2:E:208:LEU:CD1	2.45	0.45
2:F:63:MET:CE	2:F:97:VAL:HG11	2.46	0.45
1:A:286:ARG:HG2	1:A:286:ARG:NH1	2.31	0.45
1:B:171:ARG:NE	2:E:326:PHE:HB3	2.31	0.45
9:B:2003:HOH:O	2:E:124:VAL:HG13	2.16	0.45
1:C:406:PHE:HE2	2:D:393:MET:HB2	1.81	0.45
2:D:410:ILE:HG13	2:D:444:ILE:HG21	1.99	0.45
2:F:48:GLU:OE2	2:F:117:HIS:NE2	2.42	0.45
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.17	0.45
1:B:147:GLN:OE1	1:B:438:ILE:HD13	2.15	0.45
2:E:142:LEU:HG	2:E:143:LEU:HD23	1.99	0.45
2:E:227:GLY:O	2:E:231:ARG:HG2	2.16	0.45
2:F:163:THR:HG21	2:F:192:GLU:OE1	2.17	0.45
1:B:159:ILE:HG22	1:B:160:GLY:N	2.31	0.45
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.98	0.45
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:PHE:HB2	2:F:29:LEU:HD12	1.98	0.45
2:F:48:GLU:CD	2:F:117:HIS:HE2	2.24	0.45
1:A:278:TYR:HA	1:A:281:MET:CE	2.46	0.45
1:B:26:GLU:HB3	1:B:46:ASN:HD22	1.81	0.45
2:E:281:TYR:HB3	2:E:282:GLN:HE21	1.82	0.45
2:E:356:ARG:C	2:E:358:MET:H	2.25	0.45
3:G:8:ARG:O	3:G:9:ARG:C	2.58	0.45
1:B:451:GLY:C	1:B:453:LEU:H	2.25	0.45
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.99	0.45
2:F:139:VAL:HG11	2:F:348:VAL:HB	1.99	0.45
1:B:383:MET:O	1:B:384:LYS:C	2.60	0.45
1:C:75:VAL:HG12	1:C:77:GLY:H	1.80	0.45
1:C:161:ARG:NH2	1:C:197:LYS:O	2.44	0.45
2:D:27:GLU:HB2	2:D:28:GLY:H	1.63	0.45
2:F:81:PRO:O	2:F:82:ILE:C	2.59	0.45
1:B:352:LEU:HA	1:B:364:ALA:O	2.16	0.44
2:E:25:PHE:O	2:E:56:SER:HB3	2.17	0.44
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.52	0.44
2:E:94:ILE:HD11	2:E:197:TYR:CG	2.52	0.44
2:E:170:ILE:HG13	2:E:254:PHE:HE2	1.82	0.44
1:A:382:ALA:HB2	1:A:487:GLY:O	2.17	0.44
1:A:392:LEU:O	1:A:396:GLN:HG3	2.17	0.44
1:B:280:GLN:NE2	2:E:284:THR:HG22	2.33	0.44
1:B:357:PHE:HD1	1:B:358:TYR:HD1	1.65	0.44
1:C:399:GLU:CG	2:D:342:LEU:HD22	2.48	0.44
2:E:413:PHE:HB2	2:E:457:PHE:HB3	1.99	0.44
1:B:269:ASP:HA	1:B:270:ASP:HA	1.73	0.44
1:C:139:ARG:HH11	1:C:139:ARG:HD3	1.58	0.44
3:G:38:LEU:HD11	3:G:42:ARG:CZ	2.47	0.44
1:A:140:ILE:HG21	1:A:313:ASN:HA	2.00	0.44
1:C:313:ASN:OD1	1:C:313:ASN:C	2.60	0.44
1:C:440:GLU:O	1:C:444:VAL:HG13	2.16	0.44
2:D:264:ALA:O	2:D:267:GLU:HB2	2.17	0.44
2:D:402:LEU:HD11	2:D:406:ARG:HH21	1.82	0.44
2:E:289:MET:HG2	2:E:324:THR:HG22	1.98	0.44
2:F:82:ILE:O	2:F:115:ALA:HA	2.18	0.44
2:F:142:LEU:HD22	2:F:441:PHE:CD2	2.53	0.44
2:F:170:ILE:O	2:F:174:ALA:HB3	2.18	0.44
3:G:80:ALA:O	3:G:84:SER:OG	2.32	0.44
1:A:99:VAL:HG13	1:A:256:TYR:CD2	2.53	0.44
1:B:385:GLN:OE1	1:B:488:LYS:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:GLU:O	1:C:63:SER:HB2	2.17	0.44
1:C:149:GLY:HA3	1:C:435:PRO:HB3	1.99	0.44
2:D:84:ILE:CD1	2:D:95:MET:HE1	2.42	0.44
2:D:447:GLY:O	2:D:448:GLU:C	2.61	0.44
2:F:253:LEU:O	2:F:306:SER:HA	2.17	0.44
3:G:18:LYS:O	3:G:21:LYS:HB3	2.18	0.44
1:A:240:ALA:N	1:A:241:PRO:HD2	2.33	0.44
1:B:291:ARG:NH2	2:F:319:ASP:HB2	2.32	0.44
2:D:266:SER:HB3	2:D:282:GLN:NE2	2.31	0.44
2:D:381:TYR:CE1	2:D:404:VAL:HG13	2.53	0.44
2:D:402:LEU:O	2:D:406:ARG:HG3	2.18	0.44
2:F:229:ARG:HA	2:F:232:VAL:CG2	2.47	0.44
1:A:140:ILE:O	1:A:141:SER:C	2.61	0.44
1:B:393:GLU:HA	1:B:396:GLN:OE1	2.17	0.44
2:E:36:LEU:O	2:E:46:VAL:HA	2.18	0.44
2:E:292:MET:SD	2:E:293:GLN:NE2	2.90	0.44
1:A:208:GLN:O	1:A:235:THR:HG22	2.18	0.44
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.99	0.44
1:B:483:ILE:HD13	1:B:489:ILE:HG12	1.98	0.44
2:E:187:GLY:N	2:E:220:GLY:O	2.51	0.44
2:E:259:PHE:CE2	2:E:263:GLN:HG2	2.52	0.44
2:E:276:PRO:CD	3:G:266:ILE:HD11	2.38	0.44
1:B:389:THR:O	1:B:393:GLU:HG3	2.18	0.44
1:B:481:GLY:HA2	1:B:484:ARG:NH1	2.32	0.44
1:C:458:PRO:HA	1:C:461:ILE:HG13	1.98	0.44
2:E:374:VAL:O	2:E:377:ILE:HG22	2.17	0.44
2:F:460:VAL:HG23	2:F:461:GLY:N	2.33	0.44
3:G:39:LYS:N	3:G:40:PRO:CD	2.81	0.44
1:A:136:ILE:HD11	2:E:193:GLY:HA3	1.99	0.43
1:A:140:ILE:CG1	1:A:143:ARG:HH22	2.30	0.43
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.83	0.43
1:C:209:LYS:NZ	2:F:330:ASP:OD1	2.51	0.43
1:C:432:GLN:CD	4:C:600:ATP:H2'	2.43	0.43
1:C:503:ASN:O	1:C:506:ALA:HB3	2.18	0.43
2:D:406:ARG:O	2:D:410:ILE:HD12	2.18	0.43
2:F:12:ARG:HA	2:F:73:GLN:O	2.18	0.43
2:F:457:PHE:HE1	2:F:463:ILE:HD11	1.84	0.43
1:A:62:MET:CE	1:A:64:LEU:HD21	2.46	0.43
1:A:144:GLU:HA	1:A:145:PRO:HD3	1.76	0.43
1:B:32:LEU:CG	1:B:42:HIS:HB2	2.48	0.43
1:C:423:ARG:HG2	1:C:423:ARG:HH11	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:163:THR:HG23	8:E:602:PO4:O1	2.18	0.43
3:G:254:ARG:HH11	3:G:254:ARG:HD3	1.58	0.43
1:A:41:VAL:HG11	1:A:44:LEU:HD12	1.99	0.43
1:A:122:GLY:O	1:A:123:SER:C	2.61	0.43
1:B:161:ARG:NH1	1:B:198:LYS:O	2.50	0.43
1:C:438:ILE:HG23	1:C:439:GLU:N	2.33	0.43
2:D:244:ARG:HG3	2:D:304:ILE:HG13	2.00	0.43
2:E:390:ILE:C	2:E:392:GLY:H	2.26	0.43
2:E:417:PRO:HD2	2:E:460:VAL:O	2.18	0.43
1:A:209:LYS:HG2	9:A:2010:HOH:O	2.18	0.43
1:B:423:ARG:O	1:B:424:LEU:C	2.61	0.43
1:C:100:GLY:HA2	1:C:256:TYR:CD2	2.53	0.43
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.49	0.43
2:F:63:MET:HE3	2:F:97:VAL:HG11	1.99	0.43
1:A:180:ILE:HD11	1:A:216:LEU:HD22	2.01	0.43
1:C:244:TYR:CE2	1:C:281:MET:HE1	2.52	0.43
2:D:232:VAL:O	2:D:235:THR:N	2.52	0.43
2:E:142:LEU:HB2	2:E:437:THR:CG2	2.48	0.43
2:E:366:GLU:O	2:E:367:HIS:C	2.61	0.43
2:F:139:VAL:HG23	9:F:2005:HOH:O	2.17	0.43
2:F:231:ARG:O	2:F:232:VAL:C	2.62	0.43
1:B:48:GLN:HG2	2:F:70:VAL:CG2	2.49	0.43
1:C:99:VAL:HG12	1:C:100:GLY:N	2.34	0.43
2:E:170:ILE:HG13	2:E:254:PHE:CE2	2.53	0.43
2:E:454:GLU:C	2:E:456:ALA:H	2.25	0.43
2:F:36:LEU:HD13	2:F:75:VAL:HG11	2.00	0.43
3:G:24:LYS:HD2	3:G:233:ASP:HA	2.00	0.43
1:A:67:GLU:HB2	1:A:70:ASN:O	2.19	0.43
1:A:109:ASP:OD1	1:A:109:ASP:C	2.62	0.43
1:A:151:LYS:HZ1	1:A:430:GLN:HB2	1.83	0.43
1:B:444:VAL:CG1	1:B:469:LEU:HD13	2.48	0.43
1:C:30:ARG:NH2	1:C:87:ILE:HD11	2.34	0.43
2:D:188:GLU:O	2:D:222:MET:HG3	2.19	0.43
2:D:388:ILE:HD13	2:D:396:LEU:HD11	2.01	0.43
2:E:59:ARG:HD2	9:E:2003:HOH:O	2.17	0.43
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.49	0.43
2:E:111:LYS:HB2	2:E:112:GLN:OE1	2.19	0.43
1:A:210:ARG:O	1:A:211:SER:C	2.58	0.43
1:A:446:TYR:O	1:A:447:ALA:C	2.60	0.43
1:C:269:ASP:HA	1:C:270:ASP:HA	1.74	0.43
2:D:84:ILE:HB	2:D:85:PRO:CD	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:256:ASP:HA	2:D:309:ALA:HB3	2.01	0.43
2:D:468:ALA:O	2:D:469:LYS:C	2.61	0.43
2:E:384:LEU:O	2:E:388:ILE:HG12	2.19	0.43
1:B:164:ARG:HD3	1:B:164:ARG:N	2.34	0.43
1:B:288:PRO:HA	1:B:289:PRO:HD3	1.86	0.43
2:E:387:ILE:O	2:E:388:ILE:C	2.62	0.43
2:E:393:MET:HG3	2:E:396:LEU:CD1	2.49	0.43
2:F:247:GLU:HB3	2:F:249:GLN:HG2	2.01	0.43
2:F:285:LEU:C	2:F:285:LEU:HD23	2.44	0.43
1:B:94:ILE:HG21	1:B:128:ARG:HD3	2.00	0.43
1:B:142:VAL:HG12	1:B:161:ARG:O	2.19	0.43
1:C:361:ILE:O	1:C:364:ALA:HA	2.19	0.43
2:D:456:ALA:HB1	2:D:466:ALA:O	2.18	0.43
2:F:221:GLN:HA	2:F:221:GLN:HE21	1.84	0.43
1:C:30:ARG:HA	1:C:86:ASP:O	2.18	0.42
2:E:263:GLN:O	2:E:267:GLU:HG3	2.18	0.42
2:F:146:TYR:HH	2:F:333:THR:HG1	1.61	0.42
1:A:246:ALA:HB3	1:A:247:PRO:HD3	2.00	0.42
1:A:423:ARG:NH2	1:A:456:LEU:O	2.43	0.42
1:B:176:THR:O	1:B:179:ALA:N	2.52	0.42
2:D:247:GLU:C	2:D:249:GLN:H	2.26	0.42
2:D:449:TYR:HB3	2:D:452:LEU:HD12	2.01	0.42
2:F:130:GLN:HB3	2:F:357:ILE:HD11	2.01	0.42
1:A:422:VAL:HG23	1:A:423:ARG:N	2.34	0.42
1:B:323:ALA:O	1:B:324:LEU:HD23	2.20	0.42
1:C:497:LEU:O	1:C:501:VAL:HG13	2.19	0.42
2:E:167:MET:HE3	2:E:420:VAL:CG1	2.37	0.42
2:F:94:ILE:HD11	2:F:197:TYR:CG	2.54	0.42
1:A:166:LEU:CD2	1:A:168:ILE:HB	2.50	0.42
1:B:252:SER:O	1:B:255:GLU:N	2.51	0.42
1:C:48:GLN:HA	2:D:69:LEU:O	2.20	0.42
1:C:67:GLU:HB3	1:C:68:PRO:HD2	2.02	0.42
1:C:337:TYR:O	1:C:338:ILE:C	2.60	0.42
1:C:353:GLU:CD	1:C:366:ASN:HD22	2.26	0.42
1:C:356:LEU:O	1:C:357:PHE:C	2.62	0.42
2:E:96:ASN:OD1	2:E:97:VAL:N	2.52	0.42
2:E:112:GLN:NE2	2:E:242:TYR:OH	2.52	0.42
2:E:148:LYS:HE3	2:E:250:ASP:OD1	2.19	0.42
2:F:83:ARG:NH2	2:F:113:PHE:HB2	2.34	0.42
2:F:147:ALA:HB2	2:F:357:ILE:HG13	2.02	0.42
1:A:210:ARG:NH1	2:D:121:PRO:O	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:GLY:O	1:B:163:GLN:HB3	2.19	0.42
1:B:255:GLU:OE2	1:B:258:ARG:NH1	2.48	0.42
2:D:409:LYS:NZ	2:D:450:ASP:HA	2.34	0.42
2:E:89:GLU:CD	2:E:89:GLU:H	2.28	0.42
1:C:246:ALA:N	1:C:247:PRO:CD	2.83	0.42
2:E:310:ILE:CD1	2:E:329:LEU:HD11	2.49	0.42
2:F:35:ALA:O	2:F:78:SER:HB3	2.20	0.42
1:A:44:LEU:HD22	1:A:47:VAL:HG13	2.00	0.42
1:C:164:ARG:HD2	1:C:306:LEU:O	2.19	0.42
1:C:423:ARG:HH11	1:C:423:ARG:CG	2.33	0.42
2:E:456:ALA:HB1	2:E:466:ALA:O	2.20	0.42
2:F:188:GLU:C	2:F:222:MET:HE3	2.44	0.42
1:B:137:ILE:N	1:B:138:PRO:HD2	2.34	0.42
1:C:209:LYS:O	1:C:210:ARG:C	2.62	0.42
3:G:14:LYS:HA	3:G:243:ILE:HD11	2.01	0.42
1:A:164:ARG:HD3	1:A:164:ARG:N	2.35	0.42
1:B:366:ASN:O	1:B:367:VAL:C	2.62	0.42
1:B:422:VAL:O	1:B:426:GLU:HG2	2.20	0.42
2:D:9:THR:HA	2:D:27:GLU:OE1	2.20	0.42
2:E:370:VAL:O	2:E:371:ALA:C	2.63	0.42
2:F:329:LEU:HD13	2:F:332:THR:HG22	2.02	0.42
1:A:144:GLU:O	1:A:161:ARG:HG3	2.20	0.42
1:A:247:PRO:HB3	1:A:268:TYR:CD1	2.55	0.42
1:B:33:SER:HB2	2:E:52:HIS:O	2.20	0.42
1:B:191:ASP:OD1	1:B:227:LYS:NZ	2.52	0.42
1:B:251:CYS:O	1:B:255:GLU:HG3	2.20	0.42
1:C:74:VAL:CG1	1:C:241:PRO:HB3	2.50	0.42
1:C:151:LYS:NZ	1:C:427:LEU:O	2.44	0.42
2:E:387:ILE:HD12	2:E:387:ILE:N	2.33	0.42
2:F:245:ASP:C	2:F:247:GLU:N	2.77	0.42
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.50	0.42
2:F:406:ARG:O	2:F:407:ALA:C	2.61	0.42
1:B:351:PHE:HE2	1:B:353:GLU:CG	2.13	0.41
1:C:496:LYS:HD2	1:C:496:LYS:HA	1.94	0.41
2:D:372:ARG:NH1	2:D:375:GLN:OE1	2.52	0.41
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.50	0.41
1:A:102:GLU:HG3	1:A:122:GLY:C	2.45	0.41
1:A:352:LEU:HD23	1:A:365:ILE:HA	2.01	0.41
1:B:244:TYR:CD2	1:B:281:MET:HE1	2.54	0.41
1:C:213:VAL:HG12	2:F:123:PHE:CE1	2.55	0.41
1:C:213:VAL:HG12	2:F:123:PHE:HE1	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:SER:O	1:C:253:MET:HG3	2.20	0.41
1:C:300:TYR:CZ	1:C:304:ARG:HD3	2.55	0.41
2:D:118:ALA:O	2:D:295:ARG:HD2	2.20	0.41
2:D:160:VAL:CG2	2:D:335:LEU:HB3	2.50	0.41
2:E:170:ILE:HG21	2:E:215:VAL:CG2	2.49	0.41
2:E:388:ILE:CD1	2:E:396:LEU:HD11	2.50	0.41
1:A:44:LEU:HB3	1:A:47:VAL:HG22	2.02	0.41
1:B:102:GLU:HG3	1:B:122:GLY:O	2.21	0.41
1:C:362:ARG:NH2	2:F:372:ARG:HD2	2.35	0.41
2:E:210:ASP:O	2:E:212:THR:N	2.50	0.41
2:F:12:ARG:HE	2:F:74:LYS:CE	2.14	0.41
3:G:30:LYS:HD2	3:G:225:GLN:OE1	2.20	0.41
1:A:213:VAL:O	1:A:214:ALA:C	2.63	0.41
1:A:349:GLN:O	1:A:370:SER:HB3	2.20	0.41
1:A:373:ARG:NH2	9:A:2018:HOH:O	2.54	0.41
1:A:437:ALA:O	1:A:441:GLN:HG3	2.20	0.41
1:C:65:ASN:OD1	1:C:287:ARG:NH2	2.46	0.41
2:F:153:GLY:N	2:F:329:LEU:HD22	2.34	0.41
1:C:162:GLY:H	1:C:322:THR:HG1	1.67	0.41
2:E:54:GLY:O	2:E:55:GLU:HB2	2.20	0.41
2:E:160:VAL:CG1	2:E:337:ARG:HG3	2.50	0.41
2:E:189:ARG:O	2:E:190:THR:C	2.63	0.41
2:F:16:VAL:O	2:F:17:ILE:HD12	2.21	0.41
1:A:350:ILE:HA	1:A:370:SER:HB3	2.02	0.41
1:A:390:MET:CE	1:A:424:LEU:HD22	2.50	0.41
1:B:54:GLU:HG2	1:B:60:LYS:NZ	2.35	0.41
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.56	0.41
1:A:296:GLY:O	2:E:267:GLU:HB3	2.20	0.41
1:B:55:PHE:HD1	1:B:59:LEU:O	2.04	0.41
1:C:434:SER:N	1:C:435:PRO:CD	2.84	0.41
1:C:452:TYR:CD2	1:C:501:VAL:HG21	2.56	0.41
2:E:348:VAL:O	2:E:350:PRO:HD3	2.21	0.41
3:G:23:MET:HE2	3:G:232:MET:SD	2.61	0.41
1:A:239:ALA:C	1:A:241:PRO:HD2	2.46	0.41
1:A:330:GLN:O	1:A:331:ALA:C	2.63	0.41
1:A:479:LEU:HA	1:A:482:LYS:HE3	2.02	0.41
1:B:239:ALA:O	1:B:240:ALA:C	2.64	0.41
1:B:375:GLY:O	1:B:376:SER:C	2.63	0.41
1:C:287:ARG:HA	1:C:288:PRO:HD3	1.94	0.41
2:D:292:MET:HE2	2:D:292:MET:HB3	1.91	0.41
2:E:170:ILE:HG12	2:E:181:SER:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:151:LYS:NZ	2:F:293:GLN:HB3	2.35	0.41
2:F:336:SER:OG	2:F:339:ILE:HG13	2.21	0.41
2:F:378:LEU:HD21	2:F:410:ILE:HG22	2.02	0.41
1:A:139:ARG:CZ	2:E:190:THR:HG21	2.51	0.41
1:A:155:SER:OG	1:A:156:LEU:HG	2.21	0.41
1:B:209:LYS:HG3	9:B:2008:HOH:O	2.21	0.41
1:B:432:GLN:OE1	4:B:600:ATP:H2'	2.20	0.41
1:C:99:VAL:CG1	1:C:256:TYR:HB2	2.51	0.41
1:C:209:LYS:HD3	2:F:328:HIS:HA	2.01	0.41
2:D:162:LYS:N	7:D:600:ADP:O1B	2.54	0.41
2:E:136:GLY:N	2:E:141:ASP:OD2	2.51	0.41
2:E:253:LEU:O	2:E:306:SER:HA	2.21	0.41
2:E:335:LEU:HD23	2:E:335:LEU:HA	1.82	0.41
2:E:396:LEU:HB2	2:E:401:LYS:HG3	2.03	0.41
2:E:453:PRO:O	2:E:454:GLU:C	2.64	0.41
2:F:406:ARG:NH2	2:F:447:GLY:HA3	2.33	0.41
1:B:453:LEU:CD1	1:B:461:ILE:HG23	2.49	0.41
1:C:194:ASP:OD2	1:C:197:LYS:HG3	2.21	0.41
1:C:299:PHE:O	1:C:300:TYR:C	2.63	0.41
2:E:257:ASN:OD1	2:E:259:PHE:HB3	2.21	0.41
2:E:298:THR:HA	2:E:303:SER:HB2	2.02	0.41
2:E:321:ALA:HB3	2:E:322:PRO:HD3	2.03	0.41
3:G:83:SER:O	3:G:87:LYS:HG3	2.20	0.41
1:B:97:VAL:HB	1:B:98:PRO:HD2	2.03	0.40
1:B:248:TYR:CD1	6:B:701:GOL:H12	2.56	0.40
1:C:30:ARG:HG2	1:C:30:ARG:NH1	2.35	0.40
2:E:406:ARG:O	2:E:407:ALA:C	2.63	0.40
1:B:338:ILE:N	1:B:339:PRO:CD	2.84	0.40
2:E:50:ALA:C	2:E:51:GLN:HG3	2.47	0.40
2:E:93:ARG:NH2	2:E:106:GLY:O	2.39	0.40
2:E:94:ILE:HD12	2:E:103:ASP:HB3	2.03	0.40
2:F:152:ILE:C	2:F:329:LEU:HD22	2.46	0.40
2:F:370:VAL:HG21	2:F:438:ILE:HG23	2.03	0.40
1:B:62:MET:HB2	1:B:76:PHE:CE2	2.57	0.40
1:B:347:ASP:O	1:B:373:ARG:HG3	2.21	0.40
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.34	0.40
1:C:151:LYS:HG2	1:C:441:GLN:HG2	2.03	0.40
1:C:376:SER:O	1:C:378:ALA:N	2.54	0.40
2:D:83:ARG:HA	2:D:114:ALA:O	2.22	0.40
2:D:163:THR:HA	2:D:166:ILE:CG2	2.49	0.40
2:D:313:PRO:O	2:D:314:ALA:C	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:397:SER:O	2:D:401:LYS:HG2	2.21	0.40
2:D:412:ARG:C	2:D:414:LEU:H	2.29	0.40
2:F:134:VAL:CG2	2:F:434:LEU:HD22	2.51	0.40
2:F:134:VAL:HG13	2:F:141:ASP:OD1	2.21	0.40
1:A:140:ILE:HD11	1:A:143:ARG:NH2	2.27	0.40
1:B:270:ASP:HB2	1:B:326:VAL:O	2.22	0.40
1:B:393:GLU:OE1	1:B:424:LEU:HD11	2.21	0.40
1:C:190:ASN:O	1:C:198:LYS:HE3	2.21	0.40
1:C:370:SER:C	1:C:371:VAL:CG1	2.94	0.40
1:C:419:SER:O	1:C:423:ARG:HG2	2.20	0.40
2:D:48:GLU:CD	2:D:231:ARG:HE	2.25	0.40
2:E:84:ILE:HD13	2:E:235:THR:CG2	2.52	0.40
2:F:33:LEU:O	2:F:81:PRO:HB3	2.22	0.40
3:G:5:ASP:O	3:G:8:ARG:N	2.55	0.40
1:A:244:TYR:CE1	1:A:301:LEU:HD11	2.56	0.40
1:A:283:LEU:HD12	2:D:283:PRO:HB3	2.04	0.40
1:B:498:LYS:O	1:B:499:GLU:C	2.64	0.40
1:C:98:PRO:CG	1:C:112:GLY:HA3	2.51	0.40
1:C:187:LYS:HE3	1:C:224:ASP:HB3	2.02	0.40
1:C:423:ARG:HD2	1:C:461:ILE:HD11	2.01	0.40
2:E:35:ALA:HB2	2:E:82:ILE:HG13	2.04	0.40
2:E:296:ILE:HD13	2:E:306:SER:HB2	2.03	0.40
2:E:409:LYS:HD3	2:E:457:PHE:CZ	2.57	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%)	438 (90%)	38 (8%)	9 (2%)	6	23
1	B	475/510 (93%)	428 (90%)	44 (9%)	3 (1%)	21	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	490/510 (96%)	446 (91%)	42 (9%)	2 (0%)	30	59
2	D	465/482 (96%)	419 (90%)	43 (9%)	3 (1%)	21	51
2	E	464/482 (96%)	408 (88%)	50 (11%)	6 (1%)	9	32
2	F	464/482 (96%)	427 (92%)	35 (8%)	2 (0%)	30	59
3	G	116/272 (43%)	103 (89%)	9 (8%)	4 (3%)	3	12
All	All	2959/3248 (91%)	2669 (90%)	261 (9%)	29 (1%)	12	39

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	ASP
1	C	337	TYR
3	G	210	ALA
1	A	93	ALA
1	A	404	ALA
1	B	195	GLU
2	E	211	ALA
2	E	357	ILE
2	E	423	VAL
2	E	455	GLN
2	F	247	GLU
1	A	123	SER
1	A	401	ALA
1	C	405	GLN
2	D	448	GLU
2	F	246	GLN
1	A	485	THR
3	G	5	ASP
3	G	81	ILE
3	G	211	ASN
1	A	141	SER
1	A	333	ASP
1	B	187	LYS
1	B	413	ALA
2	D	247	GLU
1	A	500	ILE
2	D	279	VAL
2	E	107	PRO
2	E	170	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	354 (90%)	39 (10%)	7	24
1	B	388/412 (94%)	356 (92%)	32 (8%)	10	32
1	C	397/412 (96%)	366 (92%)	31 (8%)	11	35
2	D	377/386 (98%)	355 (94%)	22 (6%)	18	49
2	E	376/386 (97%)	350 (93%)	26 (7%)	14	41
2	F	376/386 (97%)	349 (93%)	27 (7%)	13	39
3	G	102/230 (44%)	96 (94%)	6 (6%)	18	48
All	All	2409/2624 (92%)	2226 (92%)	183 (8%)	12	36

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	45	ARG
1	A	47	VAL
1	A	50	GLU
1	A	57	SER
1	A	59	LEU
1	A	64	LEU
1	A	74	VAL
1	A	79	ASP
1	A	99	VAL
1	A	121	ILE
1	A	123	SER
1	A	129	VAL
1	A	136	ILE
1	A	140	ILE
1	A	141	SER
1	A	177	SER
1	A	211	SER
1	A	216	LEU
1	A	217	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	235	THR
1	A	249	SER
1	A	298	VAL
1	A	329	THR
1	A	338	ILE
1	A	354	THR
1	A	359	LYS
1	A	371	VAL
1	A	420	ARG
1	A	436	MET
1	A	442	VAL
1	A	444	VAL
1	A	459	SER
1	A	462	THR
1	A	472	VAL
1	A	479	LEU
1	A	489	ILE
1	A	499	GLU
1	A	505	LEU
1	B	28	THR
1	B	34	ILE
1	B	47	VAL
1	B	102	GLU
1	B	108	VAL
1	B	137	ILE
1	B	140	ILE
1	B	143	ARG
1	B	151	LYS
1	B	159	ILE
1	B	177	SER
1	B	206	ILE
1	B	209	LYS
1	B	211	SER
1	B	216	LEU
1	B	217	VAL
1	B	218	LYS
1	B	233	SER
1	B	276	VAL
1	B	298	VAL
1	B	340	THR
1	B	371	VAL
1	B	376	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	380	THR
1	B	384	LYS
1	B	389	THR
1	B	392	LEU
1	B	419	SER
1	B	434	SER
1	B	459	SER
1	B	474	SER
1	B	479	LEU
1	C	47	VAL
1	C	52	MET
1	C	57	SER
1	C	63	SER
1	C	64	LEU
1	C	65	ASN
1	C	74	VAL
1	C	123	SER
1	C	131	LEU
1	C	189	PHE
1	C	208	GLN
1	C	211	SER
1	C	217	VAL
1	C	262	LYS
1	C	267	ILE
1	C	282	SER
1	C	304	ARG
1	C	307	GLU
1	C	334	VAL
1	C	349	GLN
1	C	371	VAL
1	C	398	ARG
1	C	416	GLN
1	C	417	LEU
1	C	419	SER
1	C	423	ARG
1	C	444	VAL
1	C	474	SER
1	C	479	LEU
1	C	501	VAL
1	C	505	LEU
2	D	27	GLU
2	D	43	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	89	GLU
2	D	95	MET
2	D	97	VAL
2	D	112	GLN
2	D	127	SER
2	D	137	ILE
2	D	139	VAL
2	D	164	VAL
2	D	172	ASN
2	D	205	VAL
2	D	210	ASP
2	D	232	VAL
2	D	274	ARG
2	D	282	GLN
2	D	291	THR
2	D	303	SER
2	D	306	SER
2	D	335	LEU
2	D	403	THR
2	D	431	LEU
2	E	67	GLU
2	E	74	LYS
2	E	97	VAL
2	E	112	GLN
2	E	116	ILE
2	E	132	ILE
2	E	139	VAL
2	E	164	VAL
2	E	171	ASN
2	E	188	GLU
2	E	191	ARG
2	E	215	VAL
2	E	223	ASN
2	E	232	VAL
2	E	266	SER
2	E	279	VAL
2	E	282	GLN
2	E	297	THR
2	E	306	SER
2	E	336	SER
2	E	339	ILE
2	E	358	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	365	SER
2	E	395	GLU
2	E	431	LEU
2	E	444	ILE
2	F	17	ILE
2	F	51	GLN
2	F	67	GLU
2	F	78	SER
2	F	89	GLU
2	F	95	MET
2	F	96	ASN
2	F	97	VAL
2	F	110	THR
2	F	139	VAL
2	F	166	ILE
2	F	205	VAL
2	F	223	ASN
2	F	232	VAL
2	F	237	LEU
2	F	266	SER
2	F	274	ARG
2	F	279	VAL
2	F	282	GLN
2	F	292	MET
2	F	298	THR
2	F	303	SER
2	F	393	MET
2	F	397	SER
2	F	405	SER
2	F	420	VAL
2	F	460	VAL
3	G	2	THR
3	G	77	LEU
3	G	220	SER
3	G	226	SER
3	G	236	SER
3	G	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	466	ASN
1	B	503	ASN
1	C	260	ASN
1	C	263	HIS
1	C	349	GLN
1	C	396	GLN
1	C	405	GLN
1	C	476	HIS
2	D	130	GLN
2	D	194	ASN
2	D	198	HIS
2	D	221	GLN
2	D	282	GLN
2	D	455	GLN
2	E	34	ASN
2	E	223	ASN
2	E	246	GLN
2	E	282	GLN
2	E	293	GLN
2	E	308	GLN
2	E	375	GLN
2	E	442	GLN
2	E	455	GLN
2	F	51	GLN
2	F	221	GLN
2	F	223	ASN
2	F	249	GLN
2	F	282	GLN
2	F	411	GLN
2	F	427	HIS
2	F	443	GLN
3	G	82	HIS

5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	ATP	C	600	5	32,33,33	2.35	5 (15%)	48,52,52	1.40	7 (14%)
7	ADP	D	600	5	28,29,29	1.36	4 (14%)	43,45,45	1.10	4 (9%)
6	GOL	B	701	-	5,5,5	0.78	0	5,5,5	0.97	0
4	ATP	B	600	5	32,33,33	1.19	3 (9%)	48,52,52	1.46	8 (16%)
4	ATP	A	600	5	32,33,33	1.76	5 (15%)	48,52,52	1.50	8 (16%)
8	PO4	E	602	-	4,4,4	0.66	0	6,6,6	0.34	0
4	ATP	F	600	5	32,33,33	2.06	5 (15%)	48,52,52	0.88	2 (4%)

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	ATP	C	600	5	-	0/22/38/38	0/3/3/3
7	ADP	D	600	5	-	0/16/32/32	0/3/3/3
6	GOL	B	701	-	-	3/4/4/4	-
4	ATP	B	600	5	-	0/22/38/38	0/3/3/3
4	ATP	A	600	5	-	2/22/38/38	0/3/3/3
4	ATP	F	600	5	-	0/22/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	600	ATP	PB-O3B	8.48	1.68	1.59
4	F	600	ATP	PA-O3A	8.24	1.68	1.59
4	A	600	ATP	PB-O3B	7.42	1.67	1.59
4	C	600	ATP	PB-O3A	-6.57	1.52	1.59
4	C	600	ATP	PA-O3A	5.92	1.65	1.59
4	F	600	ATP	PB-O3B	5.81	1.65	1.59
7	D	600	ADP	PA-O3A	4.54	1.64	1.59
4	A	600	ATP	C2-N1	2.95	1.39	1.33
4	A	600	ATP	PG-O3G	-2.74	1.44	1.54
4	B	600	ATP	PB-O3B	2.68	1.62	1.59
4	B	600	ATP	C2-N1	2.56	1.38	1.33
4	B	600	ATP	PG-O3G	-2.53	1.45	1.54
4	F	600	ATP	C8-N7	2.46	1.36	1.31
7	D	600	ADP	C8-N7	2.43	1.36	1.31
4	F	600	ATP	PG-O3G	-2.31	1.46	1.54
4	A	600	ATP	O3'-C3'	2.29	1.48	1.43
4	A	600	ATP	PG-O2G	-2.26	1.46	1.54
4	C	600	ATP	PG-O3G	-2.20	1.46	1.54
7	D	600	ADP	C2-N1	2.16	1.37	1.33
4	F	600	ATP	C2-N1	2.09	1.37	1.33
4	C	600	ATP	PA-O2A	-2.04	1.45	1.55
7	D	600	ADP	PA-O2A	-2.02	1.46	1.55

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	ATP	O3'-C3'-C4'	-4.84	97.17	111.08
4	C	600	ATP	O2B-PB-O3A	4.16	118.52	107.27
4	A	600	ATP	O3'-C3'-C2'	-3.75	99.80	111.82
4	B	600	ATP	O3B-PB-O1B	3.44	121.06	110.70
4	B	600	ATP	O2B-PB-O3A	3.15	115.80	107.27
4	B	600	ATP	C4-N9-C8	3.10	109.00	105.74
4	A	600	ATP	O2B-PB-O3A	2.87	115.03	107.27
4	C	600	ATP	C2'-C1'-N9	-2.72	106.53	113.30
4	A	600	ATP	O2'-C2'-C3'	-2.72	103.09	111.82
4	C	600	ATP	C4-N9-C8	2.71	108.58	105.74
7	D	600	ADP	C4-N9-C8	2.66	108.54	105.74
7	D	600	ADP	N9-C8-N7	-2.65	110.18	113.94
4	B	600	ATP	N6-C6-N1	2.62	124.20	118.38
4	A	600	ATP	C2'-C3'-C4'	2.49	107.42	102.61
4	A	600	ATP	O3A-PA-O1A	2.37	117.83	110.70
4	C	600	ATP	O3A-PB-O1B	2.35	117.79	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	600	ATP	N6-C6-N1	2.34	123.59	118.38
4	C	600	ATP	O3'-C3'-C2'	-2.32	104.37	111.82
4	F	600	ATP	O3G-PG-O2G	2.31	116.47	107.80
4	B	600	ATP	O3A-PB-O1B	-2.30	103.78	110.70
4	B	600	ATP	C5-C4-N9	-2.27	103.33	105.81
4	C	600	ATP	O2B-PB-O1B	-2.24	102.04	112.44
4	B	600	ATP	O2A-PA-O3A	2.23	113.30	107.27
7	D	600	ADP	O3B-PB-O1B	2.15	119.20	110.83
7	D	600	ADP	N6-C6-N1	2.14	123.14	118.38
4	A	600	ATP	O2A-PA-O1A	-2.12	102.58	112.44
4	A	600	ATP	O4'-C1'-C2'	2.12	111.14	106.62
4	F	600	ATP	O3A-PA-O1A	-2.08	104.45	110.70
4	B	600	ATP	C4-C5-N7	2.01	112.88	110.58

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	701	GOL	C1-C2-C3-O3
6	B	701	GOL	O2-C2-C3-O3
4	A	600	ATP	O4'-C4'-C5'-O5'
6	B	701	GOL	O1-C1-C2-O2
4	A	600	ATP	C3'-C4'-C5'-O5'

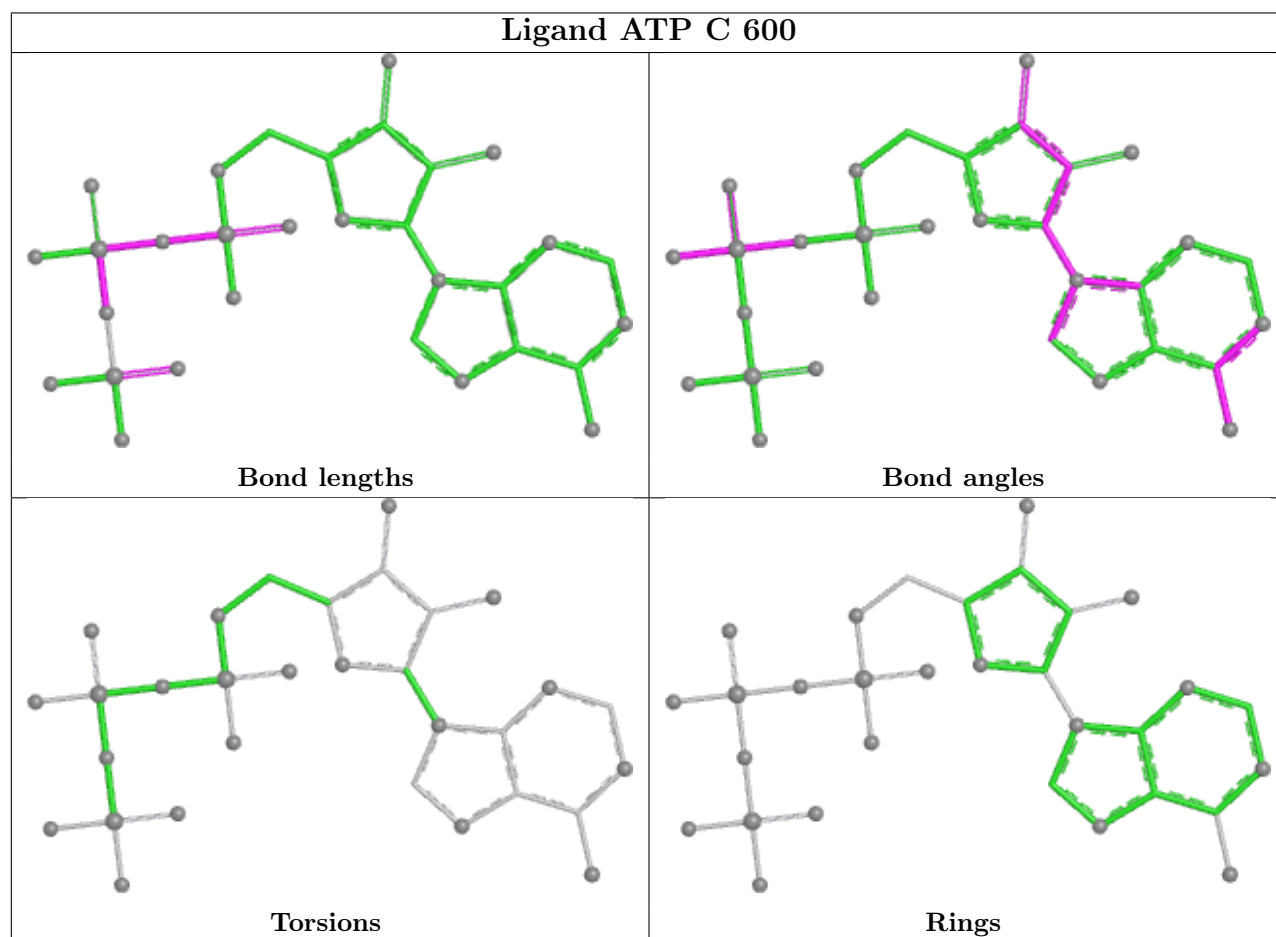
There are no ring outliers.

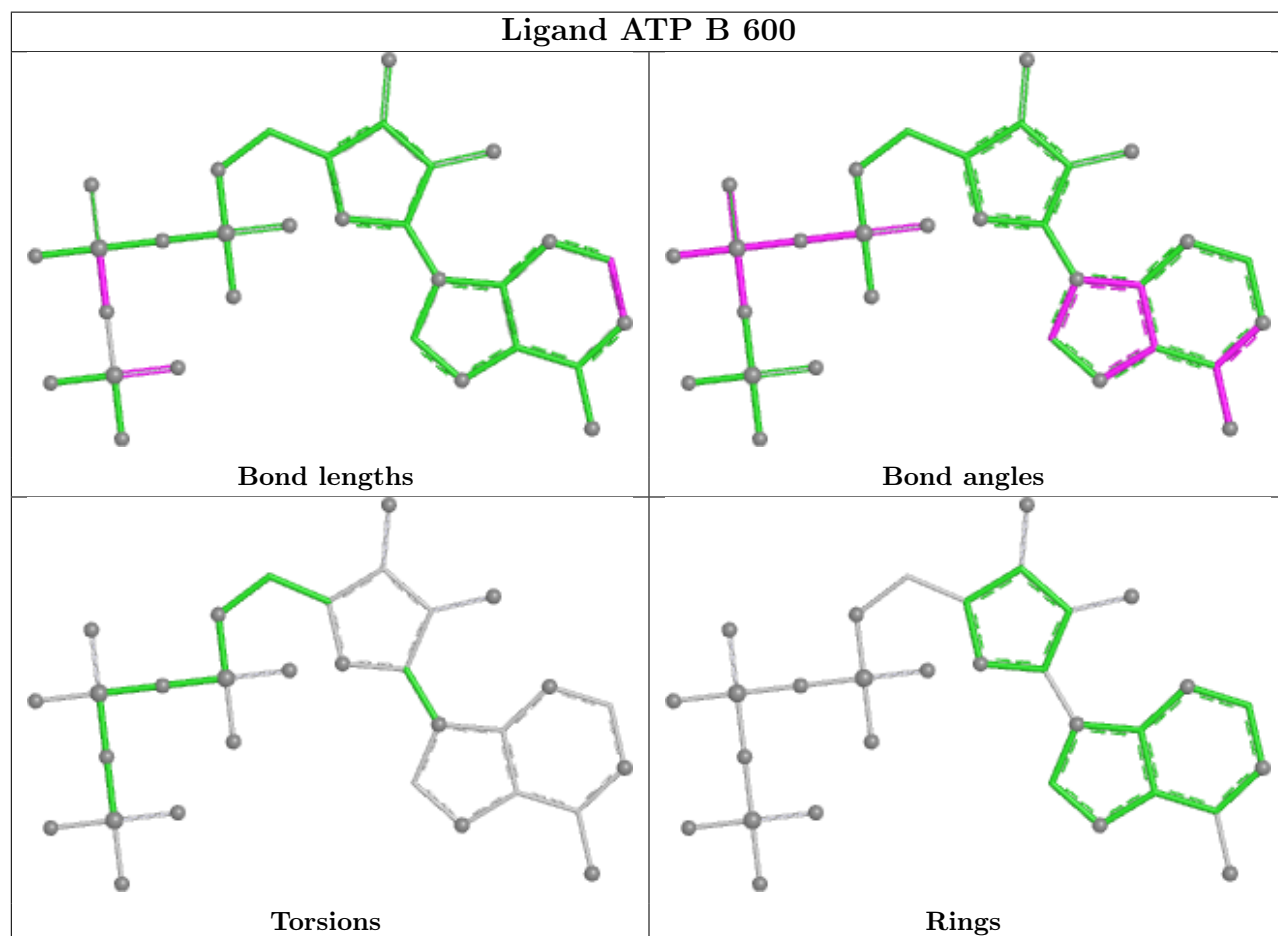
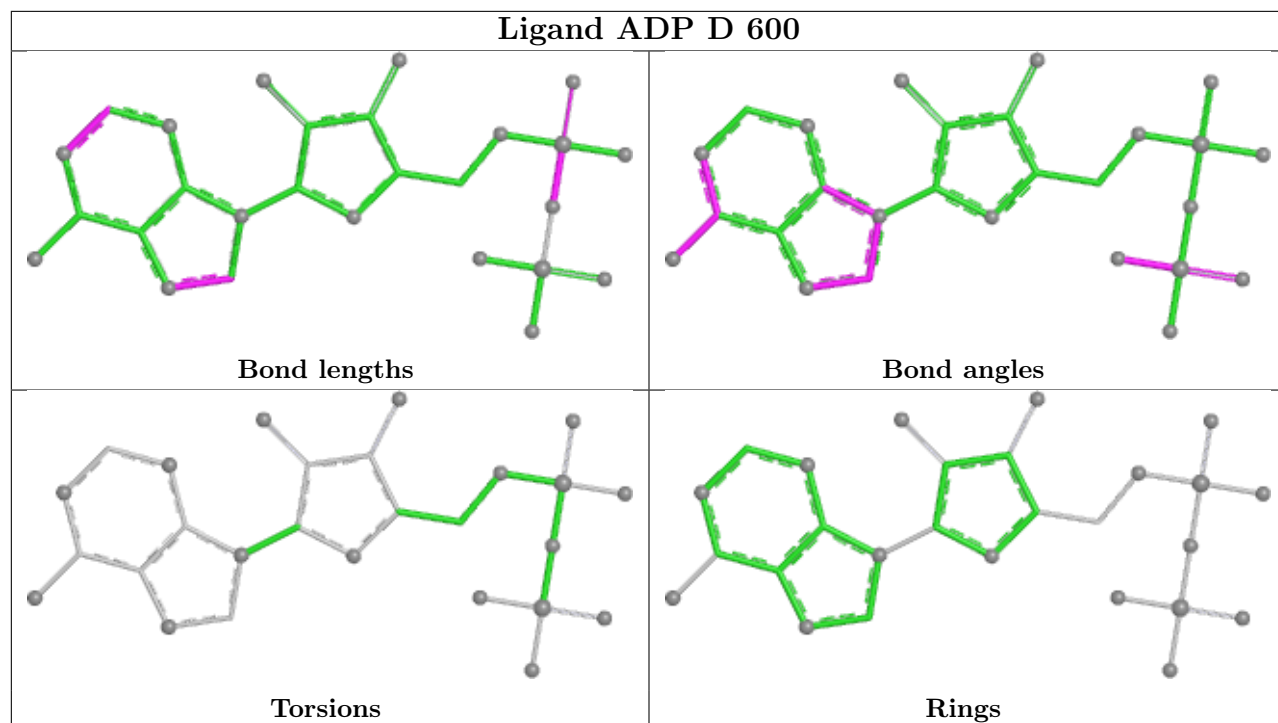
7 monomers are involved in 17 short contacts:

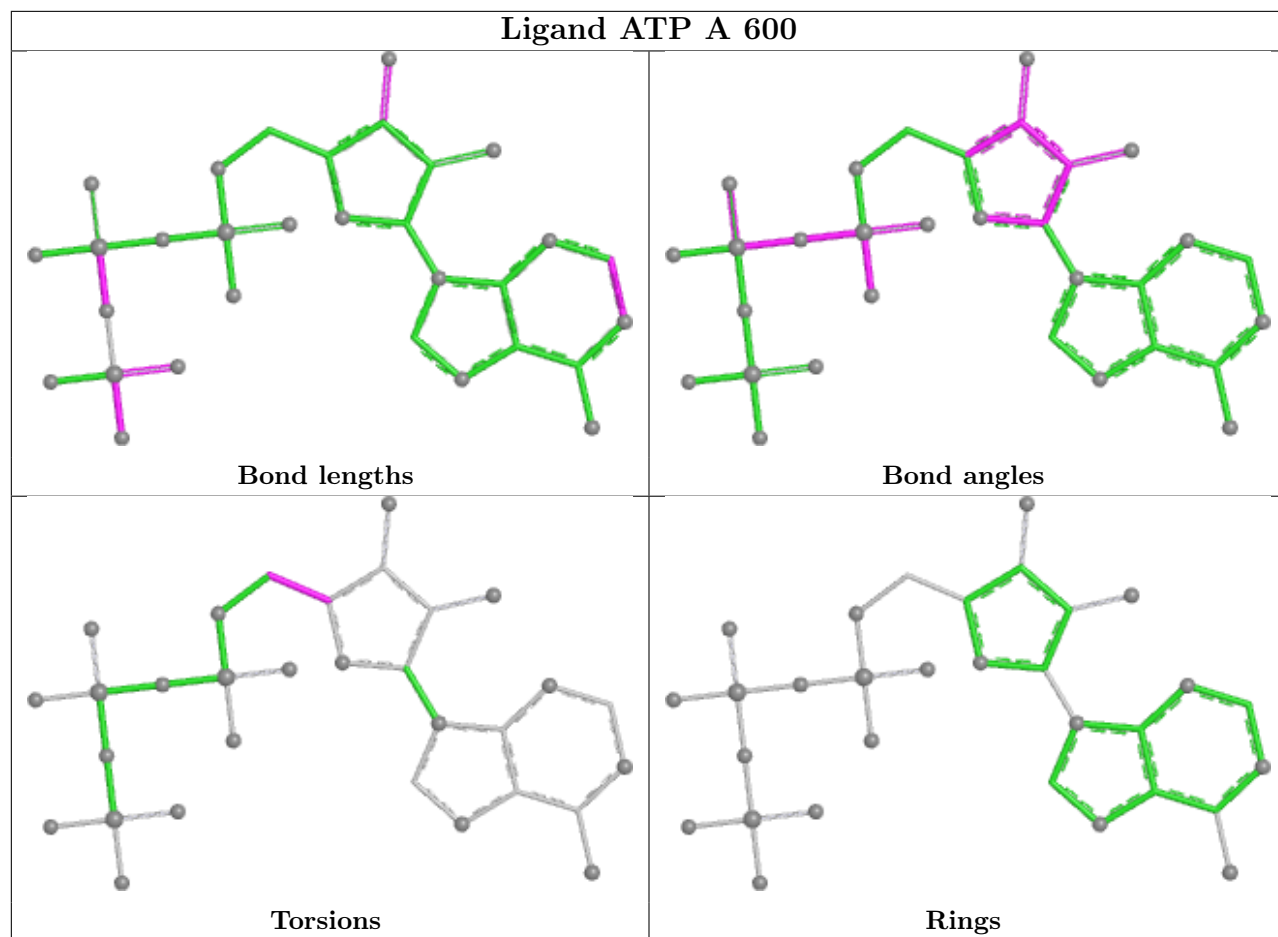
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	600	ATP	6	0
7	D	600	ADP	2	0
6	B	701	GOL	3	0
4	B	600	ATP	2	0
4	A	600	ATP	2	0
8	E	602	PO4	1	0
4	F	600	ATP	1	0

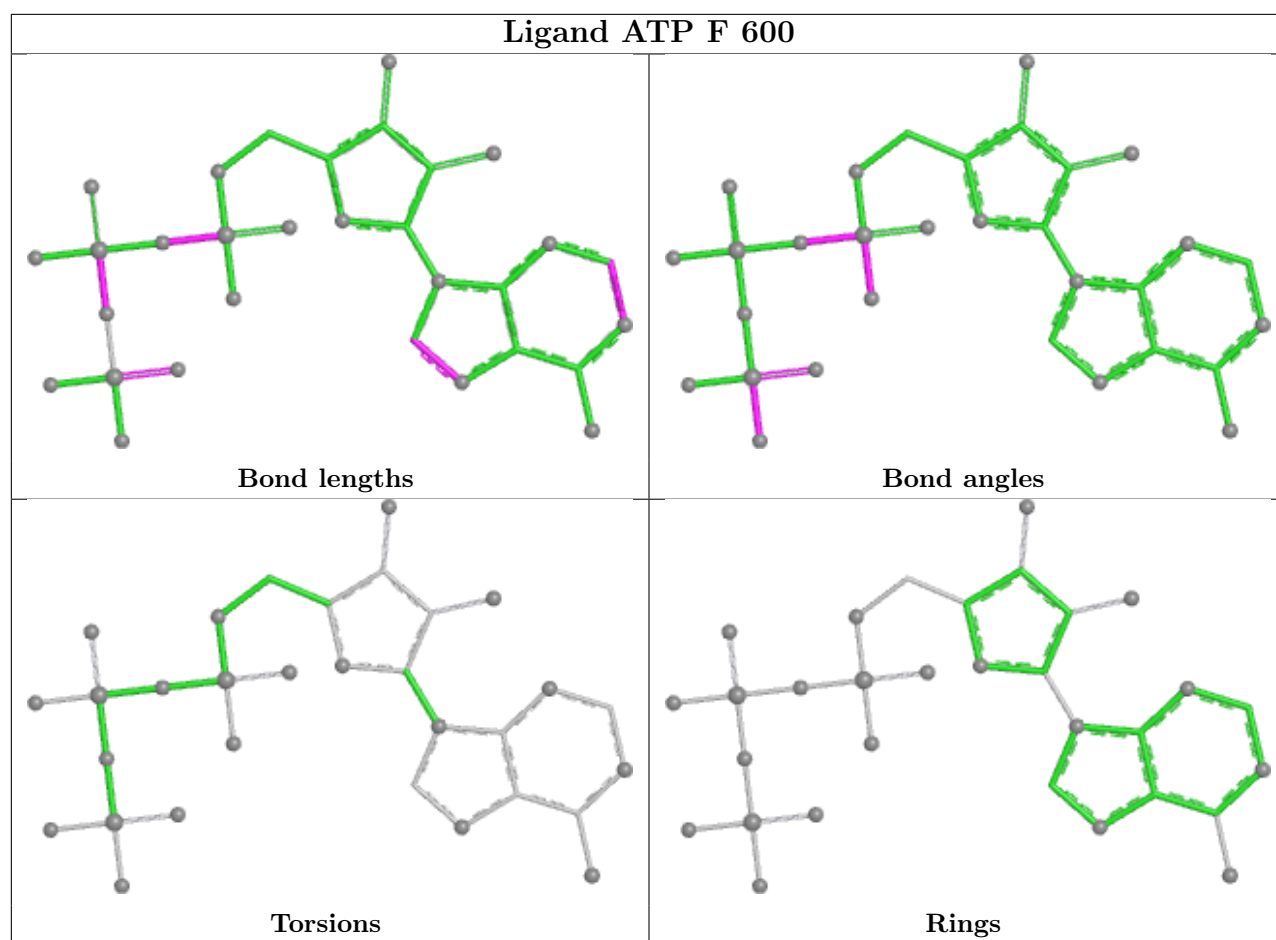
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/510 (95%)	0.04	12 (2%) 58 48	17, 41, 77, 101	0
1	B	479/510 (93%)	0.07	16 (3%) 49 40	15, 37, 89, 102	0
1	C	492/510 (96%)	-0.22	9 (1%) 67 59	15, 34, 65, 106	0
2	D	467/482 (96%)	-0.00	20 (4%) 40 31	17, 37, 77, 105	0
2	E	466/482 (96%)	0.31	26 (5%) 30 23	13, 49, 100, 114	0
2	F	466/482 (96%)	-0.07	11 (2%) 59 50	14, 36, 73, 94	0
3	G	122/272 (44%)	1.07	25 (20%) 2 2	17, 70, 100, 104	0
All	All	2979/3248 (91%)	0.06	119 (3%) 42 34	13, 40, 87, 114	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	ALA	6.3
1	A	487	GLY	5.7
2	F	474	ALA	5.5
1	B	510	ALA	4.7
3	G	209	LEU	4.7
3	G	86	ALA	4.5
2	D	474	ALA	4.4
2	F	248	GLY	4.3
3	G	223	SER	4.2
2	F	249	GLN	4.1
2	E	474	ALA	3.8
2	E	387	ILE	3.7
2	F	178	GLY	3.7
1	C	406	PHE	3.7
2	D	392	GLY	3.7
2	E	393	MET	3.7
3	G	90	LYS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	406	PHE	3.5
3	G	77	LEU	3.5
2	D	390	ILE	3.5
1	B	410	LEU	3.5
2	D	9	THR	3.5
1	B	401	ALA	3.4
2	E	473	LEU	3.4
1	C	408	SER	3.4
2	E	446	ALA	3.3
1	B	358	TYR	3.3
3	G	25	MET	3.3
2	E	391	LEU	3.3
1	A	92	GLY	3.3
2	E	470	ALA	3.3
1	B	508	PHE	3.3
1	A	94	ILE	3.2
2	D	395	GLU	3.2
2	D	396	LEU	3.1
3	G	210	ALA	3.1
3	G	29	ALA	3.1
2	F	246	GLN	3.0
1	A	381	ARG	3.0
3	G	28	ALA	3.0
2	F	386	ASP	2.9
2	F	110	THR	2.9
1	B	456	LEU	2.9
3	G	78	CYS	2.9
1	C	510	ALA	2.9
1	A	404	ALA	2.8
2	E	390	ILE	2.8
2	E	455	GLN	2.8
2	D	27	GLU	2.8
3	G	82	HIS	2.8
2	E	110	THR	2.8
3	G	211	ASN	2.8
1	A	485	THR	2.8
3	G	1	ALA	2.7
3	G	89	MET	2.7
2	E	471	ASP	2.7
1	B	509	GLU	2.7
2	D	249	GLN	2.7
1	C	410	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	112	GLN	2.6
1	C	413	ALA	2.6
1	A	488	LYS	2.6
3	G	221	THR	2.6
3	G	44	TYR	2.6
2	E	27	GLU	2.6
3	G	27	ALA	2.6
2	D	431	LEU	2.5
1	C	414	THR	2.5
1	B	412	ALA	2.5
2	E	419	GLN	2.5
2	D	473	LEU	2.4
2	E	424	PHE	2.4
1	C	488	LYS	2.4
3	G	26	VAL	2.4
2	D	202	GLU	2.4
2	D	464	GLU	2.4
3	G	38	LEU	2.4
1	C	407	GLY	2.4
2	D	247	GLU	2.4
3	G	85	VAL	2.4
2	E	438	ILE	2.4
1	B	488	LYS	2.3
3	G	83	SER	2.3
1	B	193	THR	2.3
1	B	392	LEU	2.3
2	D	110	THR	2.3
2	E	396	LEU	2.3
2	D	399	GLU	2.3
2	F	174	ALA	2.3
3	G	226	SER	2.3
2	E	423	VAL	2.3
2	D	393	MET	2.3
2	E	356	ARG	2.3
2	E	460	VAL	2.3
1	B	419	SER	2.2
2	E	388	ILE	2.2
2	F	357	ILE	2.2
1	C	105	GLY	2.2
1	B	413	ALA	2.2
1	A	407	GLY	2.2
1	B	416	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	408	SER	2.1
3	G	4	LYS	2.1
2	E	451	HIS	2.1
1	B	65	ASN	2.1
2	E	439	LYS	2.1
1	A	91	THR	2.1
2	D	400	ASP	2.1
3	G	41	ALA	2.1
2	E	427	HIS	2.1
2	E	43	THR	2.1
2	F	9	THR	2.1
2	F	176	ALA	2.1
3	G	87	LYS	2.0
2	D	402	LEU	2.0
2	D	450	ASP	2.0
1	B	455	LYS	2.0
2	E	130	GLN	2.0
2	E	466	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	D	601	1/1	0.80	0.32	38,38,38,38	0
8	PO4	E	602	5/5	0.82	0.14	80,80,81,81	0
5	MG	F	601	1/1	0.83	0.22	34,34,34,34	0
6	GOL	B	701	6/6	0.93	0.11	39,40,41,43	0
4	ATP	A	600	31/31	0.95	0.08	13,25,31,38	0

Continued on next page...

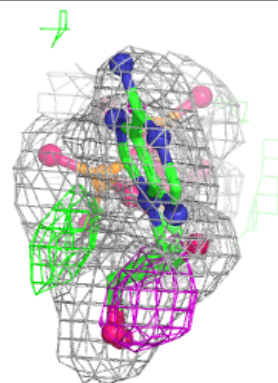
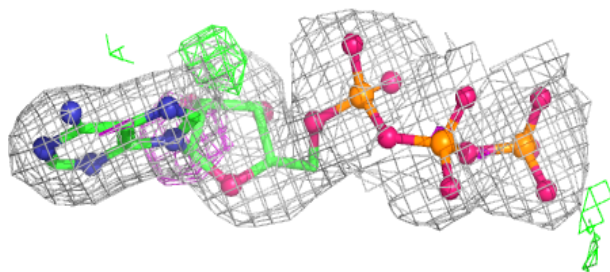
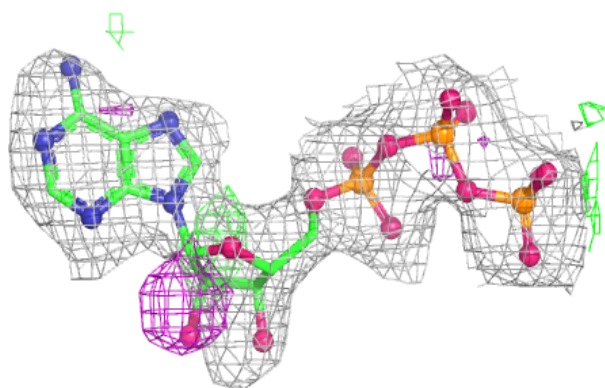
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ATP	B	600	31/31	0.95	0.09	21,28,32,38	0
5	MG	A	601	1/1	0.95	0.08	30,30,30,30	0
5	MG	C	601	1/1	0.95	0.08	23,23,23,23	0
5	MG	B	601	1/1	0.96	0.12	29,29,29,29	0
4	ATP	C	600	31/31	0.96	0.09	3,19,25,29	0
7	ADP	D	600	27/27	0.97	0.08	8,19,26,28	0
4	ATP	F	600	31/31	0.97	0.07	4,21,27,30	0

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

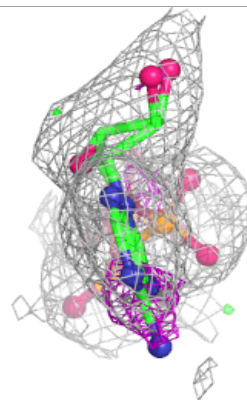
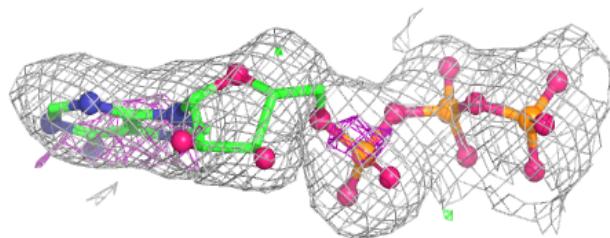
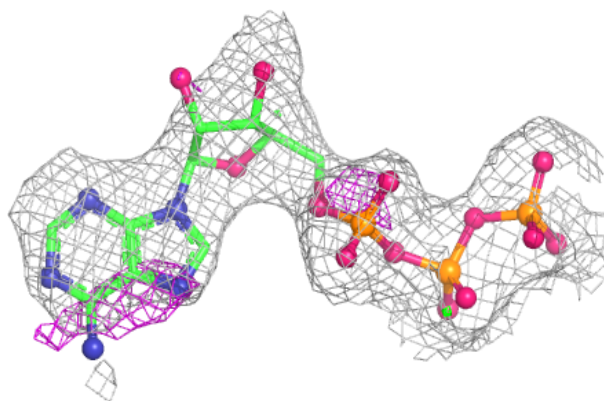
Electron density around ATP A 600:

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

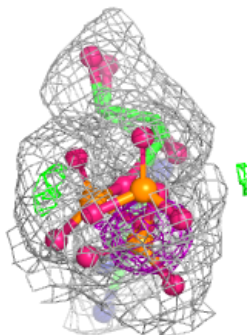
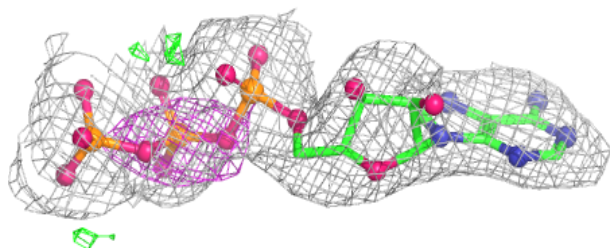
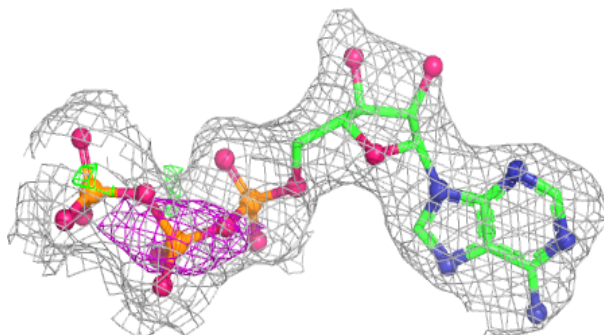


Electron density around ATP B 600:

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

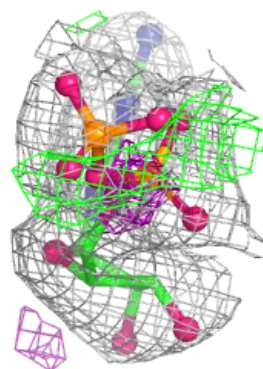
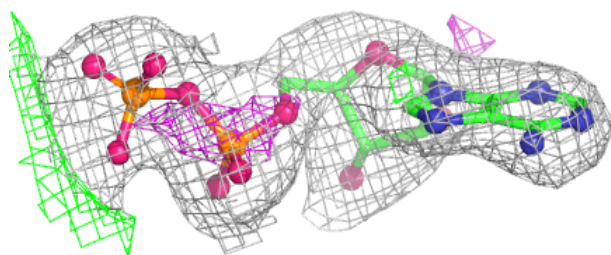
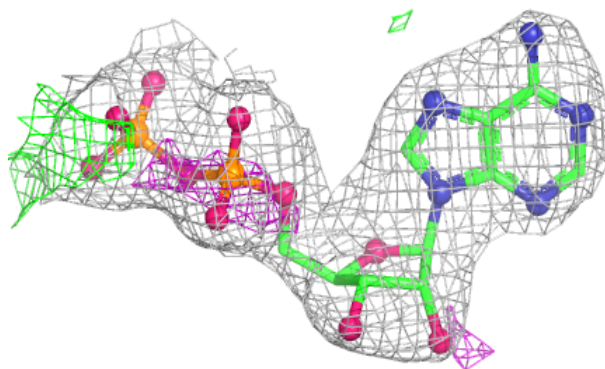
**Electron density around ATP C 600:**

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

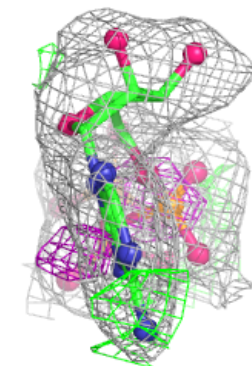
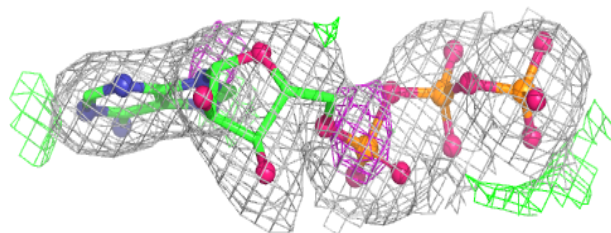
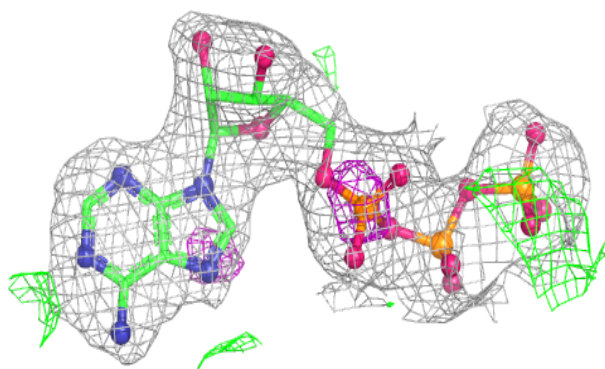


Electron density around ADP D 600:

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

**Electron density around ATP F 600:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.