



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:28 AM UTC

PDB ID : 1E1R / pdb_00001e1r
Title : BOVINE MITOCHONDRIAL F1-ATPASE INHIBITED BY MG2+ADP AND ALUMINIUM FLUORIDE
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Deposited on : 2000-05-10
Resolution : 2.50 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

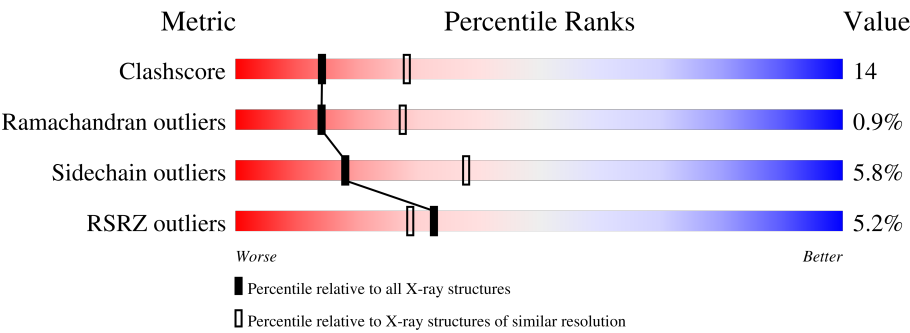
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	

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Mol	Chain	Length	Quality of chain
3	G	272	12% 32% 11% 55%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23688 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

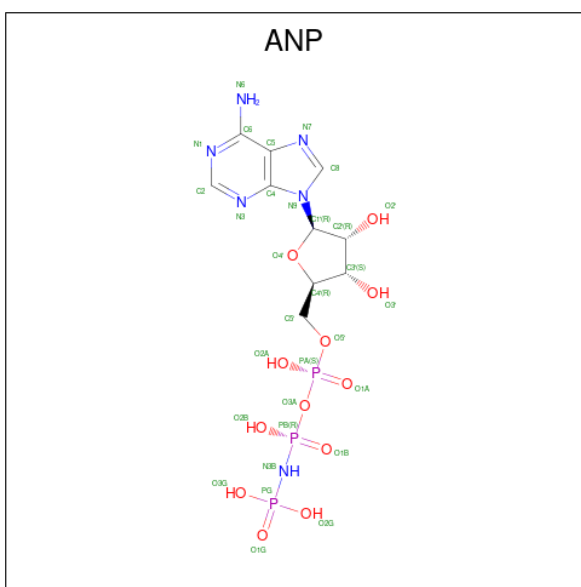
- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

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).

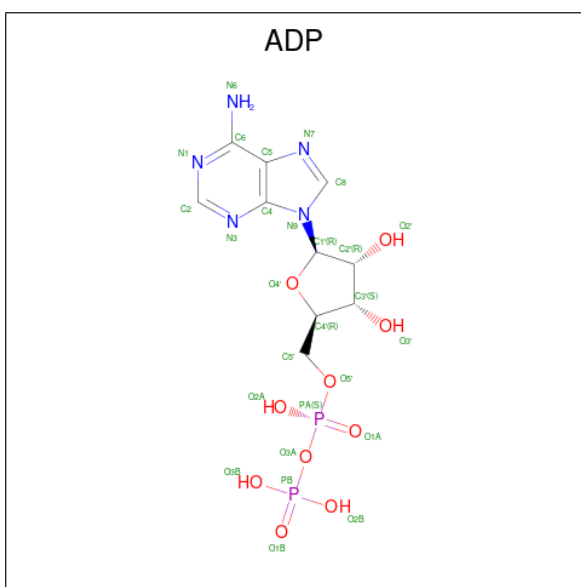


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	F	1	Total 31	C 10	N 6	O 12	P 3	0	0

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

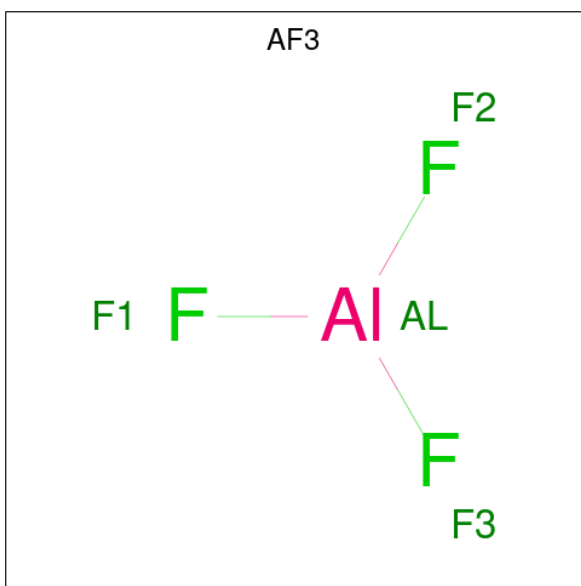
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



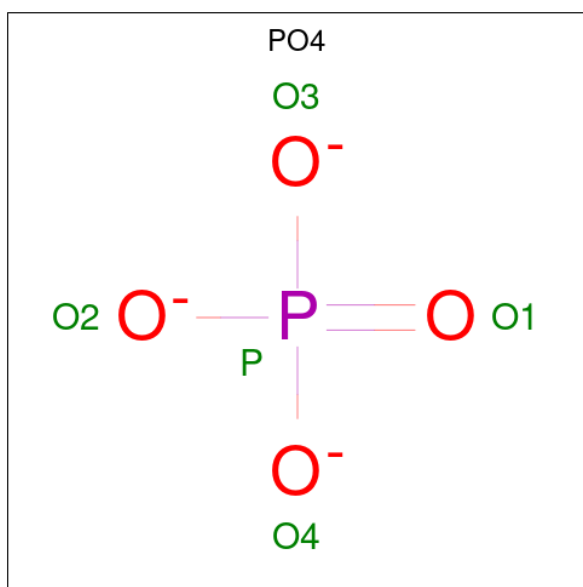
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total 4	Al 1	F 3	0	0

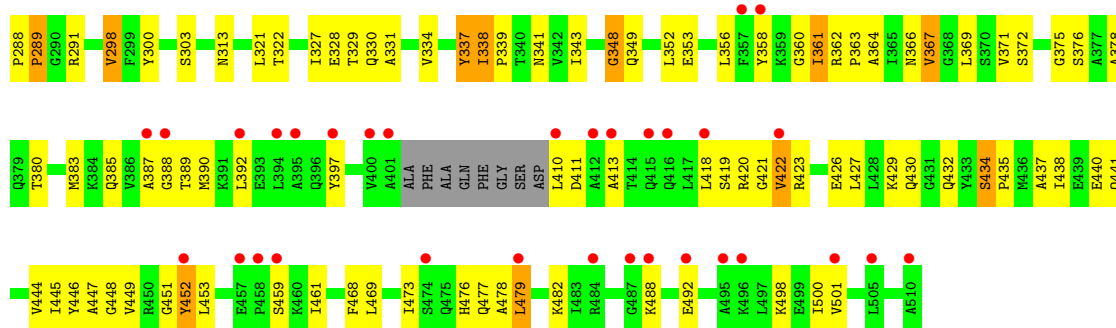
- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



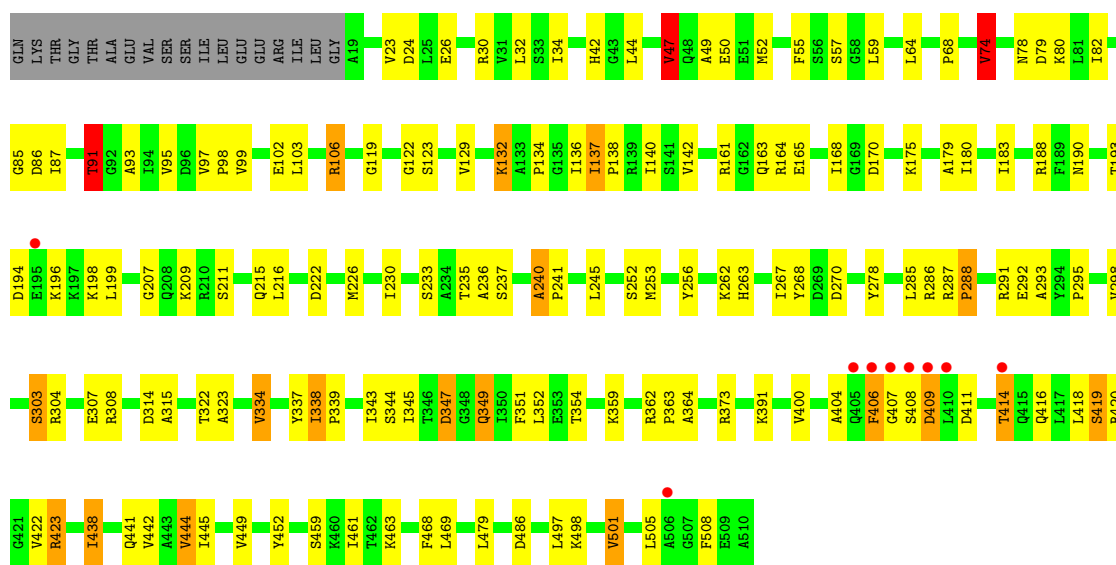
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is water.

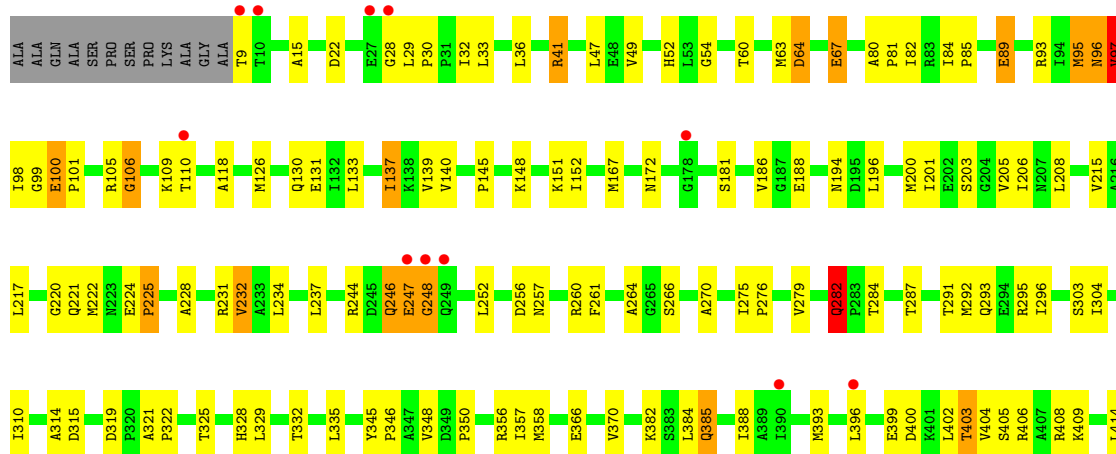
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	144	Total	O	0	0
			144	144		
9	B	126	Total	O	0	0
			126	126		
9	C	171	Total	O	0	0
			171	171		
9	D	145	Total	O	0	0
			145	145		
9	E	105	Total	O	0	0
			105	105		
9	F	148	Total	O	0	0
			148	148		
9	G	21	Total	O	0	0
			21	21		



• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

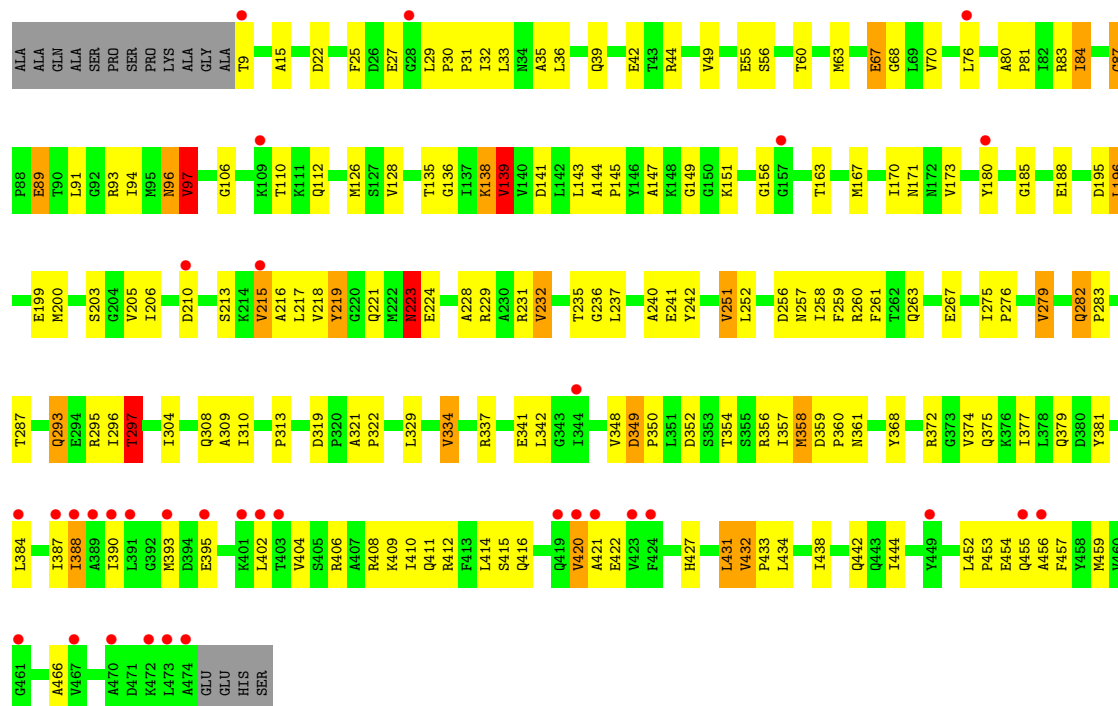


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

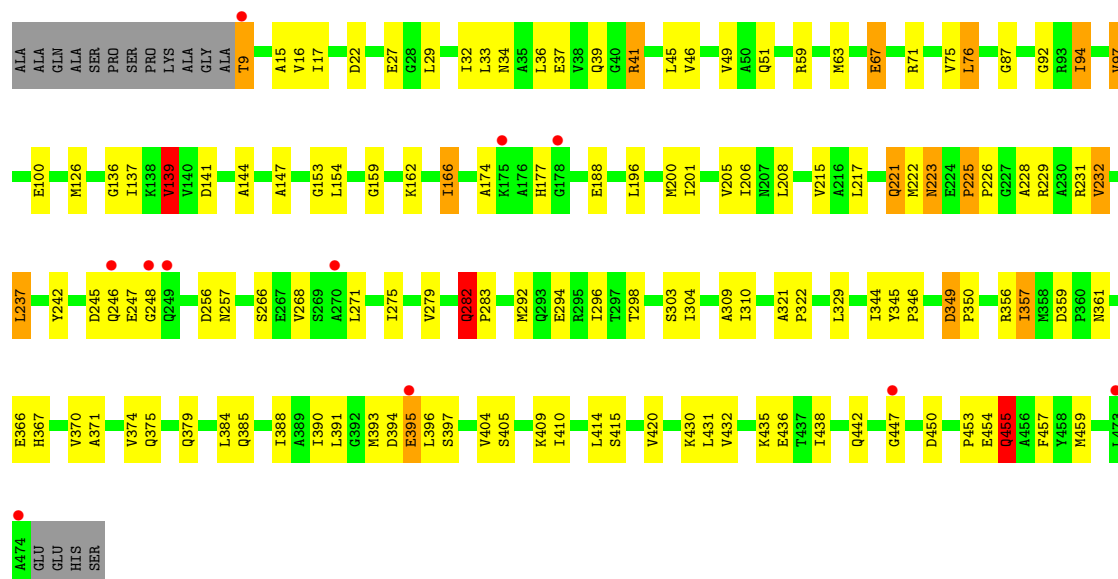




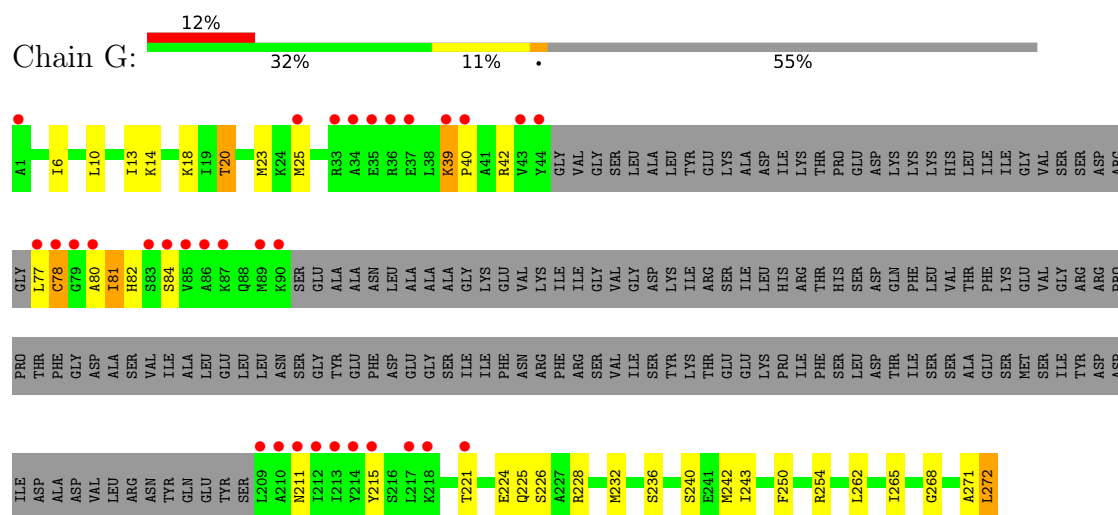
• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



• Molecule 3: 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	278.60Å 106.70Å 137.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-2.50) 95.2 (20.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.282 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23688	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, AF3, PO4, ANP, 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	0.65	0/3766	1.39	15/5080 (0.3%)
1	B	0.67	0/3704	1.41	25/4995 (0.5%)
1	C	0.71	0/3799	1.51	22/5126 (0.4%)
2	D	0.71	1/3596 (0.0%)	1.49	39/4879 (0.8%)
2	E	0.65	0/3587	1.43	30/4867 (0.6%)
2	F	0.69	0/3587	1.45	29/4867 (0.6%)
3	G	0.60	0/949	1.30	4/1266 (0.3%)
All	All	0.68	1/22988 (0.0%)	1.44	164/31080 (0.5%)

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	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	96	ASN	CA-CB	6.66	1.64	1.53

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	254	ARG	CD-NE-CZ	14.61	144.86	124.40
2	E	260	ARG	CD-NE-CZ	9.13	137.18	124.40
2	D	319	ASP	CA-CB-CG	9.04	121.64	112.60
2	D	96	ASN	CA-CB-CG	-8.88	103.72	112.60
1	C	406	PHE	CA-CB-CG	8.71	122.51	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ARG	CD-NE-CZ	8.62	136.46	124.40
1	B	140	ILE	CA-C-O	-8.32	114.26	121.09
2	D	95	MET	CA-C-N	8.09	138.29	122.03
2	D	95	MET	C-N-CA	8.09	138.29	122.03
2	D	97	VAL	CB-CA-C	-7.98	101.76	111.97
2	F	432	VAL	CA-C-O	7.91	124.33	119.19
2	E	139	VAL	N-CA-CB	7.61	118.96	110.51
2	F	41	ARG	CG-CD-NE	7.40	128.27	112.00
2	E	432	VAL	N-CA-C	7.39	115.22	107.76
2	E	97	VAL	CB-CA-C	-7.34	102.57	111.97
1	C	338	ILE	N-CA-CB	7.31	116.15	110.45
2	D	64	ASP	CA-CB-CG	7.19	119.79	112.60
1	B	348	GLY	CA-C-O	-7.09	117.19	122.37
2	F	349	ASP	CA-C-N	7.05	126.68	119.56
2	F	349	ASP	C-N-CA	7.05	126.68	119.56
2	F	144	ALA	CA-C-N	6.99	127.03	119.90
2	F	144	ALA	C-N-CA	6.99	127.03	119.90
1	B	47	VAL	CB-CA-C	-6.95	100.86	111.08
1	C	106	ARG	N-CA-C	6.87	120.17	109.52
2	E	432	VAL	CA-C-O	6.79	123.16	119.15
2	F	229	ARG	CD-NE-CZ	6.76	133.87	124.40
2	F	221	GLN	N-CA-C	6.75	119.67	110.35
1	A	157	VAL	CA-C-N	6.74	127.14	119.93
1	A	157	VAL	C-N-CA	6.74	127.14	119.93
2	D	152	ILE	CA-C-N	-6.72	117.08	121.65
2	D	152	ILE	C-N-CA	-6.72	117.08	121.65
2	E	232	VAL	CB-CA-C	-6.71	103.25	112.04
2	D	231	ARG	NE-CZ-NH2	6.71	125.24	119.20
1	C	423	ARG	CD-NE-CZ	6.71	133.79	124.40
2	E	84	ILE	N-CA-CB	-6.64	107.25	111.83
2	D	106	GLY	CA-C-N	6.60	126.57	120.03
2	D	106	GLY	C-N-CA	6.60	126.57	120.03
2	E	139	VAL	CB-CA-C	-6.58	103.45	111.88
2	E	432	VAL	CA-C-N	6.56	126.32	119.76
2	E	432	VAL	C-N-CA	6.56	126.32	119.76
2	E	144	ALA	CA-C-N	6.55	126.50	119.76
2	E	144	ALA	C-N-CA	6.55	126.50	119.76
2	D	432	VAL	CA-C-N	6.51	126.48	119.78
2	D	432	VAL	C-N-CA	6.51	126.48	119.78
2	E	223	ASN	CA-CB-CG	6.47	119.07	112.60
2	D	41	ARG	CG-CD-NE	6.47	126.22	112.00
2	F	225	PRO	CA-C-N	6.43	126.65	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	225	PRO	C-N-CA	6.43	126.65	119.32
2	E	138	LYS	CA-C-O	-6.40	114.03	121.07
2	D	96	ASN	CB-CA-C	-6.31	98.59	110.51
2	D	225	PRO	CA-C-N	6.27	126.46	119.32
2	D	225	PRO	C-N-CA	6.27	126.46	119.32
1	B	260	ASN	CA-CB-CG	-6.26	106.34	112.60
2	F	139	VAL	CB-CA-C	-6.22	104.01	111.97
2	E	349	ASP	CA-C-N	6.21	126.11	119.28
2	E	349	ASP	C-N-CA	6.21	126.11	119.28
1	A	246	ALA	CA-C-N	6.19	125.41	118.97
1	A	246	ALA	C-N-CA	6.19	125.41	118.97
2	F	357	ILE	CA-CB-CG2	6.18	121.00	110.50
2	D	282	GLN	CA-C-N	6.17	126.07	119.28
2	D	282	GLN	C-N-CA	6.17	126.07	119.28
2	E	87	GLY	CA-C-N	6.05	125.94	119.28
2	E	87	GLY	C-N-CA	6.05	125.94	119.28
1	B	167	ILE	N-CA-CB	6.04	119.29	111.67
1	C	303	SER	CA-C-N	5.92	128.22	120.28
1	C	303	SER	C-N-CA	5.92	128.22	120.28
1	C	47	VAL	CB-CA-C	-5.92	102.38	111.08
1	C	137	ILE	CA-C-N	5.91	125.58	119.56
1	C	137	ILE	C-N-CA	5.91	125.58	119.56
2	D	137	ILE	CB-CG1-CD1	5.88	126.15	113.80
2	E	297	THR	CB-CA-C	-5.88	99.80	111.91
2	F	94	ILE	CA-C-O	-5.86	114.15	120.36
1	C	240	ALA	CA-C-O	5.86	124.02	118.63
1	C	91	THR	N-CA-CB	-5.76	102.92	110.59
1	A	338	ILE	CB-CG1-CD1	5.76	125.89	113.80
2	E	334	VAL	N-CA-C	5.76	116.09	107.51
1	A	338	ILE	CA-C-N	5.73	125.41	119.05
1	A	338	ILE	C-N-CA	5.73	125.41	119.05
1	B	136	ILE	N-CA-C	5.70	116.48	110.72
1	B	47	VAL	N-CA-CB	5.68	122.63	110.64
2	E	342	LEU	N-CA-C	-5.68	106.33	113.20
2	F	141	ASP	CA-CB-CG	5.67	118.27	112.60
2	E	44	ARG	CD-NE-CZ	5.65	132.31	124.40
1	C	74	VAL	N-CA-CB	-5.64	104.57	111.00
1	B	47	VAL	O-C-N	5.63	128.42	122.62
1	A	134	PRO	N-CA-CB	5.62	108.19	103.25
1	B	287	ARG	CA-C-N	5.58	126.13	120.38
1	B	287	ARG	C-N-CA	5.58	126.13	120.38
2	D	96	ASN	CB-CG-ND2	5.57	124.75	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	PRO	N-CA-CB	5.57	108.48	103.08
2	D	105	ARG	NE-CZ-NH1	-5.56	115.94	121.50
2	D	419	GLN	CA-C-O	5.55	126.43	120.55
1	B	98	PRO	N-CA-CB	5.55	107.98	103.32
1	B	298	VAL	N-CA-CB	5.55	120.14	110.65
1	C	222	ASP	CA-C-O	-5.50	114.72	120.55
1	C	288	PRO	CA-C-N	5.48	125.75	119.83
1	C	288	PRO	C-N-CA	5.48	125.75	119.83
2	F	304	ILE	CB-CA-C	-5.48	102.98	110.77
2	E	145	PRO	N-CA-CB	5.46	108.17	103.31
2	E	223	ASN	CB-CA-C	-5.45	100.56	110.63
2	E	96	ASN	CA-CB-CG	5.43	118.03	112.60
2	E	135	THR	N-CA-C	-5.42	106.71	113.38
2	E	231	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	C	505	LEU	N-CA-C	-5.38	105.33	111.14
2	E	287	THR	CA-CB-OG1	5.37	117.66	109.60
2	F	71	ARG	CD-NE-CZ	5.37	131.91	124.40
1	B	185	ASN	CA-CB-CG	5.36	117.96	112.60
2	F	359	ASP	CA-C-N	5.32	124.99	119.56
2	F	359	ASP	C-N-CA	5.32	124.99	119.56
2	D	172	ASN	CA-CB-CG	5.30	117.90	112.60
1	A	202	ILE	CA-C-O	-5.30	114.88	120.39
1	C	349	GLN	OE1-CD-NE2	5.30	127.90	122.60
1	B	289	PRO	N-CA-CB	5.27	108.24	103.34
2	D	100	GLU	CA-C-N	5.27	125.19	119.76
2	D	100	GLU	C-N-CA	5.27	125.19	119.76
1	A	209	LYS	CA-C-N	5.27	127.59	120.38
1	A	209	LYS	C-N-CA	5.27	127.59	120.38
2	F	100	GLU	CA-C-N	5.24	125.65	119.99
2	F	100	GLU	C-N-CA	5.24	125.65	119.99
2	D	222	MET	CB-CA-C	-5.24	98.74	110.21
2	D	433	PRO	N-CA-CB	5.22	107.89	103.35
2	D	282	GLN	CB-CG-CD	5.21	121.47	112.60
2	F	282	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	B	298	VAL	CB-CA-C	-5.20	104.10	112.16
1	C	134	PRO	CA-C-O	-5.20	115.49	121.36
2	F	432	VAL	CA-C-N	5.20	124.96	119.76
2	F	432	VAL	C-N-CA	5.20	124.96	119.76
2	F	225	PRO	N-CA-CB	5.19	108.12	103.08
1	B	159	ILE	CA-CB-CG1	5.19	119.23	110.40
2	D	54	GLY	N-CA-C	-5.19	107.02	111.95
1	B	240	ALA	CA-C-N	5.18	124.98	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ALA	C-N-CA	5.18	124.98	119.28
1	C	74	VAL	O-C-N	-5.18	116.62	122.94
1	B	338	ILE	CA-C-O	5.18	122.16	118.69
1	B	337	TYR	CA-C-N	-5.17	116.20	120.33
1	B	337	TYR	C-N-CA	-5.17	116.20	120.33
2	D	101	PRO	N-CA-CB	5.16	107.91	103.31
1	A	457	GLU	CA-C-N	5.16	125.20	119.32
1	A	457	GLU	C-N-CA	5.16	125.20	119.32
2	D	261	PHE	CA-CB-CG	5.13	118.93	113.80
2	D	96	ASN	CA-C-O	-5.12	115.90	121.89
2	E	283	PRO	N-CA-CB	5.12	108.92	103.39
1	B	108	VAL	CB-CA-C	-5.09	104.21	111.19
2	F	361	ASN	CA-CB-CG	-5.09	107.51	112.60
2	F	430	LYS	CA-C-N	5.08	130.08	122.86
2	F	430	LYS	C-N-CA	5.08	130.08	122.86
2	D	252	LEU	CA-C-O	-5.08	114.84	120.38
1	C	347	ASP	CA-CB-CG	5.08	117.68	112.60
2	D	452	LEU	CA-C-N	5.07	124.83	119.76
2	D	452	LEU	C-N-CA	5.07	124.83	119.76
3	G	272	LEU	CA-C-O	-5.07	112.19	120.80
3	G	39	LYS	CA-C-N	5.05	124.55	119.19
3	G	39	LYS	C-N-CA	5.05	124.55	119.19
2	D	284	THR	CA-CB-OG1	-5.04	102.03	109.60
1	B	84	GLU	CB-CG-CD	5.04	121.17	112.60
2	F	29	LEU	CA-C-N	5.04	125.57	120.38
2	F	29	LEU	C-N-CA	5.04	125.57	120.38
1	A	145	PRO	N-CA-CB	5.03	107.78	103.31
1	A	341	ASN	OD1-CG-ND2	-5.03	117.57	122.60
2	E	219	TYR	N-CA-C	5.03	117.16	109.07
1	C	304	ARG	CA-CB-CG	5.01	124.12	114.10
1	C	486	ASP	CA-CB-CG	5.00	117.60	112.60
2	D	264	ALA	CA-C-N	5.00	125.49	119.94
2	D	264	ALA	C-N-CA	5.00	125.49	119.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	125	0
1	B	3656	0	3765	125	0
1	C	3748	0	3844	100	0
2	D	3539	0	3592	100	0
2	E	3530	0	3587	123	0
2	F	3530	0	3586	95	0
3	G	945	0	1019	22	0
4	A	31	0	13	0	0
4	B	31	0	13	4	0
4	C	31	0	13	1	0
4	F	31	0	13	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	D	27	0	12	1	0
7	D	4	0	0	1	0
8	E	5	0	0	0	0
9	A	144	0	0	6	0
9	B	126	0	0	4	0
9	C	171	0	0	4	0
9	D	145	0	0	5	0
9	E	105	0	0	3	0
9	F	148	0	0	5	0
9	G	21	0	0	1	0
All	All	23688	0	23271	656	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 14.

All (656) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:126:MET:HE1	2:E:297:THR:HG21	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:THR:HG22	1:C:93:ALA:H	1.27	1.00
1:C:211:SER:HB3	2:F:126:MET:HE2	1.42	0.99
2:F:282:GLN:H	2:F:282:GLN:HE21	0.99	0.98
2:F:166:ILE:HD11	2:F:309:ALA:HB2	1.41	0.98
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.49	0.94
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.50	0.94
2:D:282:GLN:H	2:D:282:GLN:HE21	1.11	0.93
1:A:62:MET:HE3	1:A:64:LEU:HD21	1.50	0.91
1:A:382:ALA:HB2	1:A:488:LYS:HA	1.53	0.91
1:A:440:GLU:HB3	1:A:469:LEU:HD11	1.54	0.89
2:E:293:GLN:HE22	2:E:308:GLN:HE22	1.25	0.85
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.60	0.83
2:F:282:GLN:H	2:F:282:GLN:NE2	1.77	0.83
3:G:20:THR:HG22	3:G:236:SER:HB3	1.61	0.82
2:D:139:VAL:HG12	2:D:414:LEU:HD22	1.61	0.81
2:D:388:ILE:HD12	2:D:393:MET:HE3	1.61	0.81
1:A:390:MET:HE3	1:A:424:LEU:HD22	1.64	0.80
2:F:139:VAL:HG13	2:F:414:LEU:HD22	1.64	0.80
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.64	0.80
1:C:419:SER:O	1:C:423:ARG:HG2	1.83	0.78
2:E:203:SER:HB2	2:E:420:VAL:HG22	1.64	0.78
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.66	0.78
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.66	0.78
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.65	0.78
1:A:80:LYS:HE3	2:D:33:LEU:HD12	1.66	0.77
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.66	0.77
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.65	0.77
2:D:95:MET:HE3	2:D:99:GLY:HA2	1.66	0.76
1:B:303:SER:HB2	2:F:222:MET:HB3	1.67	0.75
1:C:52:MET:O	1:C:91:THR:HB	1.86	0.74
1:A:99:VAL:HG23	1:A:253:MET:HA	1.70	0.74
1:B:390:MET:HE3	1:B:445:ILE:HG23	1.69	0.74
1:C:175:LYS:HE3	4:C:600:ANP:O1B	1.88	0.74
1:B:65:ASN:ND2	2:F:17:ILE:HG23	2.03	0.74
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.68	0.74
2:F:282:GLN:HE21	2:F:282:GLN:N	1.82	0.72
2:E:151:LYS:HE3	2:E:296:ILE:HB	1.71	0.72
1:C:423:ARG:HD2	1:C:461:ILE:HD11	1.71	0.72
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.70	0.72
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.53	0.71
2:D:282:GLN:H	2:D:282:GLN:NE2	1.87	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:223:ASN:HD22	2:F:223:ASN:H	1.36	0.71
1:C:288:PRO:HG2	2:D:270:ALA:HB1	1.73	0.71
1:C:211:SER:CB	2:F:126:MET:HE2	2.20	0.70
2:E:282:GLN:H	2:E:282:GLN:HE21	1.37	0.70
2:E:293:GLN:HA	2:E:293:GLN:HE21	1.56	0.70
2:D:408:ARG:HD3	2:D:454:GLU:OE2	1.90	0.70
1:B:479:LEU:HA	1:B:482:LYS:HD2	1.73	0.70
3:G:23:MET:SD	3:G:232:MET:HE2	2.31	0.70
2:F:405:SER:O	2:F:409:LYS:HG3	1.92	0.69
2:D:393:MET:HE1	2:D:404:VAL:HG11	1.73	0.69
2:D:200:MET:HE1	2:D:217:LEU:HD21	1.74	0.69
2:E:173:VAL:HG21	2:E:252:LEU:HD22	1.75	0.69
1:C:344:SER:HA	7:D:602:AF3:F1	1.83	0.68
2:F:200:MET:HB3	2:F:206:ILE:HG12	1.76	0.68
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.74	0.68
2:D:188:GLU:O	2:D:221:GLN:HB3	1.95	0.68
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.24	0.67
1:B:420:ARG:HH12	1:B:451:GLY:HA2	1.59	0.67
1:A:140:ILE:HG23	1:A:311:LYS:HG3	1.77	0.67
1:B:38:ILE:HG13	1:B:285:LEU:HD21	1.76	0.67
1:B:183:ILE:HD11	1:B:267:ILE:HD12	1.76	0.67
1:C:285:LEU:O	1:C:286:ARG:HB2	1.94	0.66
1:B:366:ASN:ND2	1:B:369:LEU:HD12	2.10	0.66
2:F:188:GLU:O	2:F:222:MET:HG3	1.95	0.66
2:D:366:GLU:O	2:D:370:VAL:HG23	1.96	0.65
1:A:286:ARG:HG2	1:A:286:ARG:HH11	1.61	0.65
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.79	0.65
1:A:246:ALA:HB3	1:A:247:PRO:HD3	1.79	0.64
1:B:78:ASN:HD21	1:B:80:LYS:HD3	1.62	0.64
2:D:419:GLN:O	2:D:422:GLU:HG3	1.97	0.64
2:D:384:LEU:HD22	2:D:396:LEU:HD21	1.78	0.64
2:E:388:ILE:HG23	2:E:393:MET:SD	2.38	0.64
1:A:327:ILE:HD11	1:A:342:VAL:HG21	1.79	0.64
2:F:92:GLY:HA2	2:F:206:ILE:HD12	1.80	0.64
3:G:14:LYS:HA	3:G:243:ILE:HD11	1.80	0.64
1:C:91:THR:HG22	1:C:93:ALA:N	2.08	0.63
1:C:404:ALA:C	1:C:406:PHE:H	2.05	0.63
2:D:234:LEU:CD2	2:D:292:MET:HG3	2.27	0.63
2:E:25:PHE:HB2	2:E:29:LEU:HD12	1.80	0.63
2:E:163:THR:HG21	2:E:199:GLU:OE1	1.98	0.63
2:E:375:GLN:O	2:E:379:GLN:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:MET:HE1	2:F:231:ARG:CB	2.28	0.63
1:C:418:LEU:O	1:C:422:VAL:HG23	1.98	0.62
2:E:185:GLY:HA3	2:E:188:GLU:HG2	1.82	0.62
1:B:52:MET:HG2	1:B:95:VAL:HG22	1.81	0.62
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.81	0.62
2:E:223:ASN:HD22	2:E:223:ASN:H	1.47	0.62
1:B:349:GLN:NE2	9:B:2113:HOH:O	2.33	0.61
1:C:211:SER:HB3	2:F:126:MET:CE	2.23	0.61
1:C:237:SER:HB3	2:F:294:GLU:HG3	1.82	0.61
1:C:400:VAL:HG23	1:C:418:LEU:HD21	1.82	0.61
2:F:9:THR:HG21	2:F:27:GLU:O	2.00	0.61
1:A:204:VAL:HG12	1:A:206:ILE:HD11	1.83	0.61
2:E:15:ALA:HB3	2:E:22:ASP:HB2	1.81	0.61
2:E:63:MET:CE	2:E:228:ALA:HA	2.30	0.61
1:C:463:LYS:HE2	1:C:508:PHE:CZ	2.35	0.61
1:B:419:SER:O	1:B:423:ARG:HG2	2.01	0.61
2:D:409:LYS:HD3	2:D:457:PHE:CE1	2.36	0.61
1:A:180:ILE:HD11	1:A:216:LEU:CD2	2.30	0.60
2:E:94:ILE:HG12	2:E:217:LEU:HD12	1.84	0.60
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.83	0.60
1:B:175:LYS:NZ	9:B:2122:HOH:O	2.33	0.60
1:B:175:LYS:HE3	4:B:600:ANP:O1B	2.02	0.60
2:D:139:VAL:HG11	9:D:2118:HOH:O	2.02	0.60
1:C:175:LYS:NZ	9:C:2061:HOH:O	2.34	0.60
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.32	0.60
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.02	0.59
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.37	0.59
2:F:223:ASN:HD22	2:F:223:ASN:N	1.96	0.59
2:D:205:VAL:HG12	2:D:215:VAL:HG23	1.84	0.59
2:E:89:GLU:HG3	2:E:110:THR:HA	1.85	0.59
2:F:126:MET:HE3	9:F:2039:HOH:O	2.02	0.59
2:F:223:ASN:H	2:F:223:ASN:ND2	1.96	0.59
1:A:151:LYS:HG2	1:A:441:GLN:HG2	1.83	0.59
2:E:149:GLY:HA2	2:E:304:ILE:O	2.02	0.59
2:F:275:ILE:O	2:F:283:PRO:HG3	2.02	0.59
1:A:403:PHE:HE1	3:G:18:LYS:HB3	1.65	0.59
1:C:183:ILE:HD11	1:C:267:ILE:HD13	1.84	0.59
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.83	0.59
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.85	0.59
2:E:282:GLN:H	2:E:282:GLN:NE2	2.00	0.59
1:C:359:LYS:HG3	2:F:379:GLN:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:MET:HE1	2:D:196:LEU:HD22	1.84	0.59
1:C:23:VAL:HG12	1:C:23:VAL:O	2.03	0.58
2:E:195:ASP:O	2:E:199:GLU:HB2	2.03	0.58
1:A:440:GLU:O	1:A:444:VAL:HG13	2.03	0.58
1:C:168:ILE:HD11	1:C:339:PRO:HB3	1.84	0.58
2:D:89:GLU:HG3	2:D:110:THR:HA	1.86	0.58
1:B:26:GLU:HB3	1:B:46:ASN:ND2	2.18	0.58
1:B:338:ILE:HB	1:B:339:PRO:HD3	1.86	0.58
1:A:211:SER:HB3	2:D:126:MET:HE3	1.86	0.58
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.85	0.58
1:C:44:LEU:O	1:C:47:VAL:HG22	2.03	0.58
2:F:166:ILE:HD11	2:F:309:ALA:CB	2.28	0.57
3:G:6:ILE:HG21	3:G:250:PHE:HB2	1.86	0.57
2:E:63:MET:HE3	2:E:228:ALA:HA	1.85	0.57
2:D:382:LYS:HA	2:D:385:GLN:HE21	1.69	0.57
1:A:98:PRO:HD3	1:A:126:ARG:HH21	1.67	0.57
1:A:463:LYS:HD3	1:A:508:PHE:CZ	2.39	0.57
2:E:408:ARG:HH21	2:E:412:ARG:NH2	2.02	0.57
1:A:34:ILE:HD11	1:A:79:ASP:HB2	1.86	0.57
2:E:170:ILE:HD13	2:E:215:VAL:CG2	2.34	0.57
1:C:164:ARG:HG3	1:C:323:ALA:HB3	1.86	0.57
1:B:158:PRO:O	1:B:375:GLY:HA3	2.05	0.57
2:E:49:VAL:HA	2:E:60:THR:HG22	1.87	0.57
1:A:91:THR:HA	9:A:2017:HOH:O	2.04	0.57
2:D:314:ALA:O	2:D:315:ASP:HB2	2.03	0.57
2:D:382:LYS:HA	2:D:385:GLN:NE2	2.19	0.57
1:C:24:ASP:OD2	1:C:26:GLU:HB2	2.05	0.56
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.70	0.56
2:E:334:VAL:HG21	2:E:352:ASP:HB3	1.87	0.56
1:B:141:SER:O	1:B:143:ARG:HD2	2.05	0.56
2:E:83:ARG:HD3	9:E:2018:HOH:O	2.05	0.56
2:E:223:ASN:H	2:E:223:ASN:ND2	2.02	0.56
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.70	0.56
1:A:419:SER:O	1:A:423:ARG:HD3	2.05	0.56
2:E:422:GLU:HG2	2:E:427:HIS:O	2.05	0.56
1:C:452:TYR:CD2	1:C:501:VAL:HG21	2.41	0.56
1:B:137:ILE:N	1:B:138:PRO:CD	2.69	0.56
1:B:151:LYS:HZ1	1:B:430:GLN:HB2	1.71	0.56
1:B:432:GLN:OE1	4:B:600:ANP:H2'	2.05	0.56
2:E:402:LEU:HD23	2:E:406:ARG:HH21	1.70	0.56
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:246:GLN:O	2:D:247:GLU:HG3	2.06	0.56
2:E:404:VAL:O	2:E:408:ARG:HG3	2.05	0.56
2:F:384:LEU:O	2:F:388:ILE:HG12	2.06	0.56
1:C:30:ARG:HA	1:C:86:ASP:O	2.07	0.55
1:C:52:MET:HE3	1:C:95:VAL:HG22	1.89	0.55
2:F:367:HIS:HA	2:F:438:ILE:HD12	1.88	0.55
1:B:441:GLN:O	1:B:445:ILE:HG13	2.06	0.55
1:C:411:ASP:OD1	1:C:414:THR:HG23	2.06	0.55
2:F:41:ARG:HD3	2:F:45:LEU:HD23	1.89	0.55
1:A:258:ARG:O	1:A:319:GLY:HA3	2.06	0.55
1:B:151:LYS:HE2	1:B:427:LEU:O	2.06	0.55
2:E:139:VAL:HG21	2:E:348:VAL:HB	1.89	0.55
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.71	0.55
1:A:211:SER:N	2:D:126:MET:HE2	2.22	0.55
1:A:241:PRO:O	1:A:244:TYR:HB3	2.07	0.55
2:D:93:ARG:NH2	2:D:106:GLY:O	2.40	0.55
2:D:404:VAL:O	2:D:408:ARG:HG3	2.07	0.55
2:D:474:ALA:O	2:D:475:GLU:HB2	2.07	0.55
1:C:68:PRO:HA	9:D:2001:HOH:O	2.06	0.54
2:D:145:PRO:HB2	2:D:357:ILE:HD11	1.89	0.54
2:F:228:ALA:O	2:F:232:VAL:HG22	2.07	0.54
2:D:247:GLU:O	2:D:248:GLY:C	2.50	0.54
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.43	0.54
2:E:263:GLN:O	2:E:267:GLU:HG3	2.07	0.54
1:A:293:ALA:HB2	3:G:265:ILE:HD13	1.89	0.54
1:A:184:ILE:HD12	1:A:223:ALA:HB3	1.89	0.54
1:B:78:ASN:ND2	1:B:80:LYS:HD3	2.22	0.54
1:B:246:ALA:HB3	1:B:247:PRO:HD3	1.89	0.54
1:B:151:LYS:NZ	1:B:430:GLN:HB2	2.22	0.54
1:C:52:MET:HE3	1:C:95:VAL:HG13	1.89	0.54
2:F:16:VAL:C	2:F:17:ILE:HD12	2.33	0.54
1:A:411:ASP:OD2	1:A:413:ALA:HB3	2.08	0.54
1:B:185:ASN:O	1:B:188:ARG:HD2	2.08	0.54
1:A:286:ARG:HH12	3:G:272:LEU:HD13	1.72	0.54
1:B:216:LEU:HD22	1:B:216:LEU:O	2.08	0.54
1:A:390:MET:HE2	1:A:424:LEU:HB3	1.89	0.53
2:D:36:LEU:HB2	2:D:47:LEU:HB2	1.90	0.53
2:D:266:SER:HB3	2:D:282:GLN:NE2	2.23	0.53
2:D:402:LEU:O	2:D:406:ARG:HG3	2.07	0.53
2:D:97:VAL:HG22	9:D:2062:HOH:O	2.07	0.53
2:F:345:TYR:HA	2:F:346:PRO:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:188:GLU:H	2:F:221:GLN:NE2	2.06	0.53
1:A:313:ASN:OD1	1:A:316:PHE:HD1	1.90	0.53
1:B:352:LEU:HA	1:B:364:ALA:O	2.08	0.53
2:F:147:ALA:HB2	2:F:357:ILE:HG13	1.89	0.53
2:F:154:LEU:HD12	2:F:166:ILE:HG12	1.91	0.53
2:F:438:ILE:O	2:F:442:GLN:HG3	2.08	0.53
1:A:91:THR:C	1:A:93:ALA:H	2.15	0.53
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.89	0.53
1:B:468:PHE:CE1	1:B:501:VAL:HG12	2.44	0.53
1:A:441:GLN:O	1:A:445:ILE:HG12	2.08	0.53
2:F:454:GLU:HG3	9:F:2139:HOH:O	2.08	0.53
1:B:388:GLY:O	1:B:392:LEU:HG	2.08	0.53
1:C:129:VAL:O	1:C:308:ARG:NH1	2.40	0.53
1:B:385:GLN:NE2	1:B:488:LYS:NZ	2.58	0.52
1:B:348:GLY:HA2	1:B:371:VAL:HG13	1.91	0.52
1:C:99:VAL:HG13	1:C:253:MET:HA	1.90	0.52
2:D:9:THR:HG21	2:D:28:GLY:HA3	1.91	0.52
2:F:34:ASN:O	2:F:49:VAL:HG23	2.09	0.52
2:F:201:ILE:HD13	2:F:208:LEU:HD11	1.91	0.52
1:B:172:GLN:NE2	2:E:356:ARG:NE	2.57	0.52
1:C:233:SER:OG	1:C:235:THR:HG23	2.10	0.52
2:D:200:MET:HE3	2:D:206:ILE:HD12	1.91	0.52
1:B:178:ILE:HD12	1:B:352:LEU:HD11	1.91	0.52
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.24	0.52
1:C:362:ARG:HA	1:C:363:PRO:C	2.35	0.52
1:B:286:ARG:HA	2:E:275:ILE:HD12	1.91	0.52
1:C:343:ILE:HG12	1:C:349:GLN:HG2	1.91	0.52
2:E:372:ARG:HD3	2:E:375:GLN:OE1	2.10	0.52
1:A:204:VAL:HG12	1:A:206:ILE:CD1	2.39	0.52
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.45	0.52
2:E:9:THR:HG21	2:E:27:GLU:O	2.09	0.52
2:F:393:MET:SD	2:F:404:VAL:HG11	2.50	0.52
1:C:179:ALA:HB1	1:C:267:ILE:HG12	1.92	0.52
2:D:220:GLY:CA	2:D:232:VAL:HG11	2.37	0.52
2:E:454:GLU:O	2:E:456:ALA:N	2.43	0.52
2:D:225:PRO:HB2	9:D:2013:HOH:O	2.09	0.51
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.92	0.51
1:A:48:GLN:HG2	2:E:70:VAL:CG2	2.40	0.51
1:B:44:LEU:O	1:B:47:VAL:HG22	2.11	0.51
1:B:102:GLU:HG3	1:B:123:SER:HA	1.92	0.51
2:E:32:ILE:O	2:E:33:LEU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:SER:OG	2:D:205:VAL:HG23	2.11	0.51
2:D:471:ASP:O	2:D:472:LYS:C	2.53	0.51
1:A:362:ARG:HA	1:A:363:PRO:C	2.35	0.51
1:A:347:ASP:C	1:A:373:ARG:NH1	2.69	0.51
1:C:137:ILE:HB	1:C:138:PRO:HD3	1.93	0.51
2:E:91:LEU:HD11	2:E:180:TYR:CD2	2.45	0.51
2:E:374:VAL:O	2:E:377:ILE:HG22	2.11	0.51
2:E:456:ALA:HB1	2:E:466:ALA:O	2.11	0.51
1:A:137:ILE:N	1:A:138:PRO:CD	2.74	0.50
1:B:83:LYS:HD3	2:E:31:PRO:HG3	1.91	0.50
1:B:201:CYS:O	1:B:229:THR:HA	2.11	0.50
2:E:402:LEU:HD23	2:E:406:ARG:NH2	2.26	0.50
1:A:460:LYS:N	1:A:460:LYS:HD2	2.27	0.50
1:C:103:LEU:HB2	1:C:230:ILE:HD13	1.93	0.50
1:C:240:ALA:N	1:C:241:PRO:CD	2.75	0.50
2:D:393:MET:HE2	2:D:396:LEU:HD12	1.93	0.50
2:E:170:ILE:HD13	2:E:215:VAL:HG22	1.92	0.50
2:E:237:LEU:O	2:E:241:GLU:HG3	2.10	0.50
2:E:293:GLN:HE22	2:E:308:GLN:NE2	2.02	0.50
2:F:196:LEU:HD11	2:F:200:MET:HE3	1.93	0.50
1:B:97:VAL:HG11	1:B:249:SER:HB3	1.92	0.50
1:A:99:VAL:CG2	1:A:253:MET:HA	2.38	0.50
1:A:106:ARG:NH2	1:A:119:GLY:O	2.39	0.50
2:D:151:LYS:HE2	2:D:328:HIS:O	2.12	0.50
2:D:348:VAL:O	2:D:350:PRO:HD3	2.12	0.50
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.41	0.50
1:B:426:GLU:OE1	1:B:429:LYS:HE3	2.12	0.50
1:A:134:PRO:HD3	9:A:2030:HOH:O	2.11	0.50
1:A:40:ARG:NH1	9:A:2004:HOH:O	2.44	0.49
1:A:45:ARG:NH2	1:A:68:PRO:O	2.44	0.49
1:A:185:ASN:OD1	1:A:435:PRO:HB2	2.12	0.49
1:A:292:GLU:O	1:A:293:ALA:HB3	2.10	0.49
2:F:51:GLN:HG2	2:F:59:ARG:HB3	1.94	0.49
2:F:206:ILE:HD11	2:F:215:VAL:HB	1.95	0.49
2:F:371:ALA:O	2:F:375:GLN:HG3	2.11	0.49
1:B:52:MET:HE1	1:B:111:LEU:CD2	2.42	0.49
2:F:174:ALA:O	2:F:177:HIS:HB3	2.13	0.49
3:G:221:THR:O	3:G:225:GLN:HG2	2.12	0.49
1:B:362:ARG:HA	1:B:363:PRO:C	2.36	0.49
1:C:400:VAL:HG23	1:C:418:LEU:CD2	2.41	0.49
2:E:147:ALA:HA	2:E:357:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:293:GLN:NE2	2:E:308:GLN:HE22	2.02	0.49
2:E:310:ILE:HD11	2:E:329:LEU:HD11	1.94	0.49
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.95	0.49
2:D:287:THR:O	2:D:291:THR:HG23	2.13	0.49
2:D:399:GLU:O	2:D:403:THR:HG23	2.13	0.49
2:F:395:GLU:OE1	3:G:77:LEU:HD23	2.12	0.49
1:A:400:VAL:HG13	1:A:403:PHE:CD2	2.47	0.49
1:A:466:ASN:O	1:A:470:SER:OG	2.30	0.49
1:B:99:VAL:HG11	1:B:256:TYR:HB2	1.95	0.49
3:G:78:CYS:HG	3:G:82:HIS:CD2	2.30	0.49
1:C:354:THR:HG23	9:C:2128:HOH:O	2.12	0.49
2:D:133:LEU:HB2	2:D:148:LYS:HG2	1.95	0.49
2:F:97:VAL:HG13	2:F:232:VAL:HG13	1.95	0.49
1:A:347:ASP:C	1:A:373:ARG:HH11	2.21	0.49
1:A:307:GLU:HG3	2:E:223:ASN:ND2	2.27	0.49
2:D:393:MET:CE	2:D:404:VAL:HG11	2.42	0.49
2:F:226:PRO:HB2	2:F:268:VAL:HG13	1.94	0.49
1:A:180:ILE:O	1:A:184:ILE:HG12	2.13	0.48
9:A:2007:HOH:O	2:E:67:GLU:HG3	2.12	0.48
1:C:292:GLU:O	1:C:293:ALA:HB3	2.12	0.48
1:B:103:LEU:HD12	1:B:103:LEU:N	2.28	0.48
1:C:170:ASP:O	1:C:175:LYS:HE2	2.13	0.48
2:D:400:ASP:O	2:D:404:VAL:HG23	2.12	0.48
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.95	0.48
2:E:358:MET:HE1	2:E:368:TYR:CD1	2.48	0.48
1:C:400:VAL:HG13	9:C:2143:HOH:O	2.12	0.48
2:E:224:GLU:O	2:E:229:ARG:NH1	2.45	0.48
1:B:94:ILE:O	1:B:95:VAL:C	2.57	0.48
2:D:200:MET:HE3	2:D:206:ILE:CD1	2.43	0.48
1:A:136:ILE:HD13	2:E:94:ILE:HD13	1.95	0.48
1:C:55:PHE:CE1	1:C:82:ILE:HD13	2.49	0.48
2:D:405:SER:O	2:D:409:LYS:HG3	2.14	0.48
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.44	0.48
2:F:321:ALA:CB	2:F:322:PRO:CD	2.89	0.48
1:A:27:GLU:O	1:A:90:ARG:HG3	2.13	0.48
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.95	0.48
1:B:383:MET:SD	1:B:387:ALA:HB2	2.53	0.48
1:C:102:GLU:HG2	1:C:122:GLY:O	2.13	0.48
1:C:163:GLN:HG3	1:C:347:ASP:HB2	1.95	0.48
2:E:390:ILE:HG13	3:G:25:MET:SD	2.54	0.48
1:B:105:GLY:HA2	1:B:226:MET:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:VAL:HG22	1:B:372:SER:N	2.28	0.48
1:B:397:TYR:HD1	1:B:418:LEU:HA	1.79	0.48
2:F:36:LEU:HB3	2:F:75:VAL:CG1	2.43	0.48
2:F:453:PRO:O	2:F:454:GLU:C	2.57	0.48
1:C:268:TYR:O	1:C:270:ASP:HA	2.13	0.48
1:A:36:ASP:O	1:A:284:LEU:HD13	2.14	0.48
1:A:456:LEU:HD12	1:A:457:GLU:H	1.78	0.48
1:B:289:PRO:HD2	9:G:2021:HOH:O	2.14	0.48
2:E:163:THR:O	2:E:167:MET:HG3	2.14	0.48
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.95	0.48
2:F:32:ILE:O	2:F:33:LEU:HB2	2.13	0.48
1:C:438:ILE:O	1:C:442:VAL:HG23	2.13	0.47
2:D:310:ILE:HD13	2:D:325:THR:HG21	1.96	0.47
9:C:2011:HOH:O	2:D:67:GLU:HG2	2.14	0.47
2:F:153:GLY:HA3	2:F:329:LEU:HD13	1.96	0.47
1:B:411:ASP:OD2	1:B:413:ALA:HB3	2.14	0.47
2:F:388:ILE:HD12	2:F:393:MET:HG2	1.95	0.47
1:B:156:LEU:HD13	1:B:367:VAL:HG13	1.97	0.47
2:F:17:ILE:HG22	2:F:271:LEU:HD22	1.95	0.47
2:F:390:ILE:HG22	2:F:391:LEU:HD23	1.96	0.47
1:B:151:LYS:HG2	1:B:441:GLN:HG2	1.95	0.47
2:F:385:GLN:NE2	9:F:2124:HOH:O	2.47	0.47
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.95	0.47
1:A:224:ASP:O	1:A:227:LYS:HE3	2.13	0.47
1:A:327:ILE:HD12	1:A:338:ILE:HG22	1.96	0.47
1:B:300:TYR:HA	1:B:303:SER:OG	2.14	0.47
1:C:32:LEU:HD21	1:C:42:HIS:HB2	1.97	0.47
2:F:37:GLU:OE2	2:F:46:VAL:HG22	2.15	0.47
1:A:468:PHE:O	1:A:472:VAL:HG13	2.14	0.47
1:B:145:PRO:HG3	1:B:378:ALA:O	2.14	0.47
1:B:169:GLY:O	1:B:328:GLU:HA	2.15	0.47
1:B:170:ASP:O	1:B:175:LYS:HE2	2.14	0.47
1:C:52:MET:CE	1:C:95:VAL:HG13	2.45	0.47
2:D:205:VAL:CG1	2:D:215:VAL:HG23	2.43	0.47
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.44	0.47
2:F:154:LEU:CD1	2:F:166:ILE:HG12	2.44	0.47
2:F:409:LYS:HD3	2:F:457:PHE:CE2	2.49	0.47
2:D:96:ASN:HB2	2:D:100:GLU:O	2.15	0.47
1:A:427:LEU:HD11	1:A:448:GLY:HA3	1.97	0.47
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.50	0.47
2:E:84:ILE:HG21	2:E:235:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:337:ARG:O	2:E:341:GLU:HG3	2.15	0.47
1:B:157:VAL:O	1:B:159:ILE:HD13	2.14	0.47
2:E:97:VAL:HG21	2:E:228:ALA:HB1	1.97	0.47
1:A:137:ILE:N	1:A:138:PRO:HD3	2.30	0.46
1:A:145:PRO:HB2	1:A:147:GLN:HE21	1.80	0.46
2:E:167:MET:HE3	2:E:420:VAL:HG11	1.96	0.46
1:A:106:ARG:NH1	1:A:121:ILE:HG22	2.31	0.46
1:C:97:VAL:HB	1:C:98:PRO:HD2	1.96	0.46
2:D:32:ILE:O	2:D:33:LEU:HB2	2.15	0.46
2:D:388:ILE:CD1	2:D:393:MET:HE3	2.40	0.46
2:E:438:ILE:O	2:E:442:GLN:HB2	2.15	0.46
1:A:48:GLN:HB3	2:E:68:GLY:HA2	1.98	0.46
1:A:175:LYS:HB2	1:A:175:LYS:HE2	1.71	0.46
1:C:99:VAL:CG1	1:C:256:TYR:HB2	2.45	0.46
2:E:87:GLY:HA2	2:E:242:TYR:CE1	2.51	0.46
1:B:385:GLN:NE2	1:B:488:LYS:HZ3	2.13	0.46
1:C:80:LYS:HA	2:F:32:ILE:HB	1.97	0.46
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.98	0.46
2:F:159:GLY:HA2	4:F:600:ANP:HNB1	1.80	0.46
1:B:102:GLU:CG	1:B:123:SER:HA	2.45	0.46
2:E:256:ASP:HA	2:E:257:ASN:HA	1.67	0.46
2:E:456:ALA:O	2:E:466:ALA:HA	2.16	0.46
2:F:266:SER:HB3	2:F:282:GLN:HE22	1.80	0.46
1:A:157:VAL:N	1:A:158:PRO:CD	2.79	0.46
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.98	0.46
1:B:434:SER:N	1:B:435:PRO:HD3	2.30	0.46
1:B:476:HIS:CE1	1:B:500:ILE:HG12	2.51	0.46
1:C:414:THR:O	1:C:418:LEU:HG	2.16	0.46
2:E:384:LEU:O	2:E:388:ILE:HG12	2.16	0.46
2:F:292:MET:HE3	2:F:292:MET:HB3	1.84	0.46
1:C:441:GLN:O	1:C:445:ILE:HG12	2.16	0.46
2:D:63:MET:CE	2:D:228:ALA:HA	2.46	0.46
2:D:131:GLU:HB3	9:D:2037:HOH:O	2.15	0.46
1:B:32:LEU:HG	1:B:42:HIS:HB2	1.97	0.46
1:B:40:ARG:NH1	9:B:2003:HOH:O	2.48	0.46
1:A:338:ILE:N	1:A:339:PRO:CD	2.79	0.46
1:C:132:LYS:HE3	2:D:224:GLU:OE2	2.16	0.46
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.98	0.46
2:D:439:LYS:O	2:D:443:GLN:HG3	2.16	0.46
2:E:409:LYS:HG2	2:E:457:PHE:CE1	2.50	0.46
1:A:49:ALA:O	1:A:50:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLU:CD	1:A:439:GLU:H	2.24	0.45
1:B:240:ALA:N	1:B:241:PRO:CD	2.78	0.45
1:B:390:MET:HB2	1:B:449:VAL:HG21	1.98	0.45
1:A:443:ALA:O	1:A:446:TYR:HB3	2.16	0.45
1:B:343:ILE:HG12	1:B:349:GLN:HG2	1.97	0.45
2:D:329:LEU:HD12	2:D:332:THR:HG22	1.97	0.45
2:E:138:LYS:HE3	2:E:416:GLN:HB2	1.98	0.45
2:E:147:ALA:HB2	2:E:357:ILE:HG21	1.98	0.45
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.82	0.45
2:F:245:ASP:C	2:F:247:GLU:H	2.24	0.45
1:A:268:TYR:CZ	1:A:305:LEU:HD11	2.52	0.45
1:A:278:TYR:CD2	1:A:301:LEU:HD13	2.52	0.45
1:B:52:MET:HE1	1:B:111:LEU:HD22	1.97	0.45
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.52	0.45
2:D:49:VAL:HA	2:D:60:THR:HG22	1.99	0.45
1:A:62:MET:CE	1:A:64:LEU:HD21	2.35	0.45
1:A:136:ILE:HG22	9:E:2049:HOH:O	2.17	0.45
1:A:245:LEU:O	1:A:246:ALA:C	2.59	0.45
2:D:345:TYR:HA	2:D:346:PRO:C	2.41	0.45
2:E:409:LYS:HG2	2:E:457:PHE:CD1	2.52	0.45
1:B:432:GLN:HG3	4:B:600:ANP:C5	2.47	0.45
2:D:130:GLN:HE22	2:D:356:ARG:HG2	1.82	0.45
2:F:447:GLY:HA2	2:F:450:ASP:OD1	2.17	0.45
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.99	0.45
1:A:476:HIS:CD2	1:A:500:ILE:HD11	2.51	0.45
1:B:452:TYR:OH	1:B:498:LYS:HG3	2.17	0.45
2:E:258:ILE:O	2:E:261:PHE:HB3	2.17	0.45
3:G:10:LEU:O	3:G:14:LYS:HG3	2.16	0.45
1:B:64:LEU:HG	1:B:65:ASN:ND2	2.31	0.45
1:B:100:GLY:O	1:B:103:LEU:HD13	2.17	0.45
1:B:353:GLU:CD	1:B:366:ASN:HD22	2.24	0.45
1:C:132:LYS:NZ	2:D:64:ASP:OD1	2.50	0.45
1:C:420:ARG:HH11	1:C:420:ARG:HG2	1.82	0.45
2:E:96:ASN:OD1	2:E:97:VAL:HG23	2.16	0.45
2:E:411:GLN:HG3	9:E:2101:HOH:O	2.16	0.45
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.98	0.45
2:E:55:GLU:O	2:E:56:SER:HB2	2.16	0.45
1:A:104:LEU:HD22	1:A:228:TYR:C	2.43	0.44
1:A:338:ILE:N	1:A:339:PRO:HD2	2.32	0.44
1:A:422:VAL:HG23	1:A:423:ARG:HD2	1.99	0.44
1:A:422:VAL:HG23	1:A:423:ARG:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ARG:NH2	1:A:494:ASP:OD1	2.50	0.44
1:C:338:ILE:N	1:C:339:PRO:CD	2.80	0.44
1:C:352:LEU:HA	1:C:364:ALA:O	2.17	0.44
2:F:87:GLY:HA2	2:F:242:TYR:CE1	2.51	0.44
2:E:39:GLN:NE2	2:E:76:LEU:HG	2.33	0.44
2:E:63:MET:HE1	2:E:228:ALA:HA	1.97	0.44
2:E:258:ILE:HD12	2:E:258:ILE:HA	1.86	0.44
2:E:387:ILE:N	2:E:387:ILE:HD12	2.32	0.44
2:F:225:PRO:CB	2:F:226:PRO:HD2	2.47	0.44
1:C:408:SER:O	1:C:409:ASP:C	2.60	0.44
2:E:141:ASP:HB3	2:E:434:LEU:HD13	2.00	0.44
2:E:275:ILE:HA	2:E:276:PRO:HD3	1.74	0.44
2:F:162:LYS:O	2:F:166:ILE:HG13	2.17	0.44
1:A:213:VAL:O	1:A:216:LEU:HB3	2.18	0.44
1:B:28:THR:HG23	1:B:89:LYS:HG2	1.99	0.44
1:B:356:LEU:HB3	1:B:361:ILE:HB	2.00	0.44
2:E:200:MET:HB3	2:E:206:ILE:HG13	1.98	0.44
2:E:251:VAL:HG12	2:E:252:LEU:N	2.32	0.44
2:E:349:ASP:HA	2:E:350:PRO:HD2	1.79	0.44
2:F:247:GLU:O	2:F:248:GLY:C	2.60	0.44
1:B:140:ILE:HG13	1:B:141:SER:N	2.33	0.44
1:B:358:TYR:C	1:B:360:GLY:H	2.26	0.44
2:D:63:MET:CE	2:D:97:VAL:HG11	2.48	0.44
2:D:463:ILE:HD12	2:D:466:ALA:HB3	2.00	0.44
2:E:91:LEU:HD23	2:E:216:ALA:HB2	2.00	0.44
2:E:218:VAL:HG21	2:E:236:GLY:HA2	1.97	0.44
2:F:94:ILE:HG12	2:F:217:LEU:HD12	1.99	0.44
2:F:256:ASP:HA	2:F:257:ASN:HA	1.76	0.44
2:E:188:GLU:O	2:E:221:GLN:HA	2.18	0.44
2:E:263:GLN:HA	2:E:263:GLN:NE2	2.33	0.44
1:A:95:VAL:HG11	1:A:245:LEU:HD13	1.99	0.44
1:B:52:MET:O	1:B:91:THR:HG23	2.18	0.44
1:B:420:ARG:NH1	1:B:448:GLY:O	2.51	0.44
1:C:85:GLY:O	1:C:86:ASP:C	2.60	0.44
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.99	0.44
2:E:432:VAL:HA	2:E:433:PRO:HD3	1.80	0.44
1:A:441:GLN:O	1:A:444:VAL:HG22	2.18	0.43
1:B:97:VAL:HB	1:B:98:PRO:HD2	1.99	0.43
1:B:329:THR:HG21	1:B:334:VAL:HG12	1.99	0.43
1:C:199:LEU:HD12	1:C:263:HIS:O	2.18	0.43
1:C:303:SER:HA	1:C:345:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.53	0.43
2:E:360:PRO:HD3	2:E:368:TYR:CE1	2.53	0.43
2:F:455:GLN:H	2:F:455:GLN:CD	2.24	0.43
1:A:37:GLY:HA2	9:A:2012:HOH:O	2.17	0.43
2:D:82:ILE:HD13	2:D:98:ILE:HG22	2.00	0.43
1:B:50:GLU:O	1:B:95:VAL:HG23	2.19	0.43
1:B:269:ASP:HA	1:B:270:ASP:HA	1.41	0.43
1:C:207:GLY:O	1:C:236:ALA:HB2	2.18	0.43
2:F:39:GLN:CD	2:F:76:LEU:HD22	2.43	0.43
2:F:394:ASP:CG	3:G:80:ALA:HB2	2.43	0.43
1:B:249:SER:O	1:B:253:MET:HG3	2.18	0.43
1:B:446:TYR:O	1:B:447:ALA:C	2.60	0.43
1:C:49:ALA:O	1:C:50:GLU:HB2	2.18	0.43
2:D:256:ASP:HA	2:D:257:ASN:HA	1.81	0.43
1:A:204:VAL:CG1	1:A:206:ILE:HD11	2.46	0.43
1:B:59:LEU:HD12	1:B:59:LEU:HA	1.90	0.43
1:C:452:TYR:OH	1:C:498:LYS:HG3	2.18	0.43
1:C:468:PHE:CE1	1:C:501:VAL:HG12	2.53	0.43
1:A:240:ALA:N	1:A:241:PRO:CD	2.82	0.43
1:A:311:LYS:NZ	1:A:318:GLY:O	2.49	0.43
1:A:355:GLU:O	1:A:359:LYS:HB2	2.19	0.43
1:B:38:ILE:HG13	1:B:285:LEU:CD2	2.47	0.43
1:B:161:ARG:HA	1:B:322:THR:OG1	2.19	0.43
1:B:473:ILE:O	1:B:477:GLN:HG2	2.18	0.43
1:C:137:ILE:N	1:C:138:PRO:CD	2.81	0.43
2:D:151:LYS:NZ	2:D:293:GLN:O	2.52	0.43
2:D:275:ILE:HG23	2:D:276:PRO:HD2	2.00	0.43
1:A:244:TYR:CE1	1:A:301:LEU:HD11	2.52	0.43
1:B:206:ILE:HG21	1:B:274:GLN:HB2	2.00	0.43
1:B:410:LEU:O	1:B:411:ASP:HB3	2.18	0.43
1:C:444:VAL:HG23	1:C:445:ILE:HD13	2.01	0.43
2:F:9:THR:O	2:F:76:LEU:HD12	2.18	0.43
1:B:422:VAL:O	1:B:426:GLU:HG2	2.19	0.43
1:C:129:VAL:HA	1:C:252:SER:OG	2.19	0.43
1:C:168:ILE:HD13	1:C:334:VAL:HG12	2.01	0.43
2:E:381:TYR:CE1	2:E:404:VAL:HG13	2.53	0.43
1:B:338:ILE:O	1:B:341:ASN:HB2	2.17	0.43
1:B:444:VAL:CG1	1:B:469:LEU:HD13	2.48	0.43
2:D:97:VAL:HG13	2:D:232:VAL:HG13	2.01	0.43
2:E:196:LEU:HD23	2:E:219:TYR:OH	2.18	0.43
1:C:163:GLN:O	1:C:322:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:MET:HE1	1:B:445:ILE:HD12	2.01	0.42
1:C:74:VAL:CG1	1:C:241:PRO:HB3	2.48	0.42
3:G:42:ARG:HA	3:G:215:TYR:HE1	1.83	0.42
1:A:121:ILE:HD13	1:A:121:ILE:H	1.83	0.42
2:D:84:ILE:HD12	2:D:95:MET:HE1	2.01	0.42
2:F:459:MET:HG3	9:F:2141:HOH:O	2.19	0.42
1:A:268:TYR:HB2	1:A:325:PRO:HA	2.02	0.42
1:A:446:TYR:CD2	1:A:497:LEU:HD13	2.54	0.42
1:B:28:THR:CG2	1:B:87:ILE:HG23	2.50	0.42
1:B:291:ARG:HB3	1:B:337:TYR:CD2	2.54	0.42
1:C:106:ARG:NH2	1:C:119:GLY:O	2.44	0.42
9:B:2010:HOH:O	2:F:67:GLU:HG2	2.18	0.42
2:D:244:ARG:HD3	2:D:304:ILE:HG13	2.01	0.42
2:E:257:ASN:HB2	2:E:309:ALA:O	2.20	0.42
2:F:275:ILE:HD13	3:G:271:ALA:HB1	2.01	0.42
2:F:374:VAL:HG13	2:F:410:ILE:HG21	1.99	0.42
2:F:409:LYS:NZ	2:F:450:ASP:HA	2.34	0.42
1:B:453:LEU:HD13	1:B:461:ILE:HD12	2.01	0.42
2:D:234:LEU:HD23	2:D:292:MET:HG3	2.00	0.42
2:E:352:ASP:O	2:E:354:THR:HG23	2.20	0.42
2:F:17:ILE:CG2	2:F:271:LEU:HD22	2.49	0.42
1:A:44:LEU:O	1:A:47:VAL:HG22	2.20	0.42
1:C:194:ASP:OD1	1:C:196:LYS:HB2	2.19	0.42
2:D:29:LEU:HA	2:D:30:PRO:HD2	1.87	0.42
2:E:408:ARG:NH2	2:E:412:ARG:NH2	2.66	0.42
1:A:128:ARG:HB3	1:A:131:LEU:HD21	2.01	0.42
1:B:338:ILE:N	1:B:339:PRO:CD	2.82	0.42
1:C:373:ARG:HA	6:D:600:ADP:O3'	2.20	0.42
2:E:93:ARG:NH2	2:E:106:GLY:O	2.39	0.42
1:A:40:ARG:HD2	1:A:70:ASN:OD1	2.19	0.42
1:A:151:LYS:CE	1:A:427:LEU:O	2.67	0.42
1:A:407:GLY:HA3	1:A:410:LEU:CD1	2.50	0.42
1:B:54:GLU:HG2	1:B:60:LYS:NZ	2.35	0.42
1:B:180:ILE:HD12	1:B:216:LEU:HD21	2.02	0.42
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.02	0.42
2:D:139:VAL:HG23	2:D:140:VAL:N	2.34	0.42
2:E:167:MET:HE3	2:E:420:VAL:CG1	2.50	0.42
3:G:78:CYS:SG	3:G:228:ARG:NH2	2.92	0.42
1:B:51:GLU:HA	1:B:94:ILE:HA	2.01	0.42
2:E:30:PRO:HA	2:E:31:PRO:HD3	1.85	0.42
2:E:200:MET:HG2	2:E:205:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:374:VAL:HG13	2:E:410:ILE:HG21	2.02	0.42
1:A:336:ALA:HB3	1:A:339:PRO:HG2	2.01	0.42
1:B:218:LYS:HG2	2:E:128:VAL:HB	2.02	0.42
2:D:80:ALA:HB1	2:D:81:PRO:HD2	2.02	0.42
2:D:276:PRO:HG3	3:G:268:GLY:HA3	2.01	0.42
2:F:349:ASP:HA	2:F:350:PRO:HD2	1.89	0.42
1:A:390:MET:HG3	1:A:424:LEU:HD13	2.02	0.41
1:C:91:THR:CG2	1:C:93:ALA:HB3	2.49	0.41
2:E:143:LEU:HD22	2:E:375:GLN:HG3	2.02	0.41
2:E:319:ASP:HB3	2:E:322:PRO:HD2	2.02	0.41
2:E:454:GLU:C	2:E:456:ALA:N	2.78	0.41
1:B:174:GLY:HA2	4:B:600:ANP:PA	2.60	0.41
2:E:452:LEU:HB3	2:E:453:PRO:HD2	2.01	0.41
1:A:24:ASP:OD2	1:A:27:GLU:HB2	2.19	0.41
1:C:314:ASP:O	1:C:315:ALA:C	2.62	0.41
2:E:411:GLN:HA	2:E:414:LEU:HD12	2.03	0.41
2:E:421:ALA:O	2:E:422:GLU:C	2.62	0.41
2:F:201:ILE:CD1	2:F:208:LEU:HD11	2.50	0.41
3:G:20:THR:HA	3:G:232:MET:HE3	2.02	0.41
1:A:34:ILE:HD11	1:A:79:ASP:CB	2.51	0.41
1:B:157:VAL:N	1:B:158:PRO:CD	2.84	0.41
1:A:34:ILE:CG2	2:D:52:HIS:HB2	2.51	0.41
1:A:175:LYS:CG	1:A:352:LEU:HD12	2.51	0.41
1:B:313:ASN:C	1:B:313:ASN:OD1	2.64	0.41
1:C:142:VAL:HG13	1:C:161:ARG:O	2.20	0.41
2:D:118:ALA:O	2:D:295:ARG:HD2	2.20	0.41
2:D:434:LEU:O	2:D:438:ILE:HG13	2.20	0.41
2:E:359:ASP:OD2	2:E:361:ASN:HB2	2.21	0.41
3:G:39:LYS:HB2	3:G:40:PRO:CD	2.34	0.41
1:B:330:GLN:O	1:B:331:ALA:C	2.63	0.41
1:C:291:ARG:HD3	1:C:337:TYR:CE1	2.55	0.41
2:D:417:PRO:HB3	2:D:459:MET:CE	2.51	0.41
1:A:285:LEU:O	1:A:286:ARG:HB2	2.21	0.41
1:B:28:THR:HG22	1:B:87:ILE:HG23	2.01	0.41
1:C:68:PRO:HD3	2:D:15:ALA:HB2	2.03	0.41
2:F:393:MET:HE2	9:F:2125:HOH:O	2.19	0.41
1:A:248:TYR:CE1	1:A:305:LEU:HB2	2.55	0.41
1:A:335:SER:HB2	9:A:2103:HOH:O	2.19	0.41
2:F:435:LYS:HG3	2:F:436:GLU:N	2.35	0.41
3:G:81:ILE:HG13	3:G:224:GLU:HA	2.03	0.41
1:A:140:ILE:CG2	1:A:311:LYS:HG3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:TYR:CE2	1:A:497:LEU:HB3	2.56	0.41
1:B:166:LEU:HD11	1:B:327:ILE:HB	2.03	0.41
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.84	0.41
2:E:321:ALA:N	2:E:322:PRO:HD2	2.36	0.41
3:G:13:ILE:HD13	3:G:242:MET:SD	2.61	0.41
1:A:40:ARG:HD3	1:A:40:ARG:HA	1.89	0.41
1:A:152:ALA:HA	1:A:428:LEU:HD22	2.03	0.41
1:C:404:ALA:C	1:C:406:PHE:N	2.74	0.41
1:C:497:LEU:O	1:C:501:VAL:HG13	2.21	0.41
2:D:139:VAL:HG12	2:D:414:LEU:CD2	2.42	0.41
2:E:240:ALA:O	2:E:251:VAL:HG21	2.20	0.41
2:E:35:ALA:O	2:E:36:LEU:HD23	2.21	0.40
1:B:173:THR:O	1:B:352:LEU:HD13	2.22	0.40
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.84	0.40
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	0.40
2:D:417:PRO:HB3	2:D:459:MET:HE1	2.03	0.40
1:A:301:LEU:HD23	1:A:302:HIS:CD2	2.56	0.40
1:B:478:ALA:O	1:B:482:LYS:HG3	2.22	0.40
1:C:136:ILE:HG23	2:D:194:ASN:HA	2.04	0.40
1:C:287:ARG:HA	1:C:288:PRO:HD3	1.88	0.40
1:C:406:PHE:O	1:C:408:SER:N	2.55	0.40
2:D:84:ILE:HB	2:D:85:PRO:HD2	2.03	0.40
2:E:251:VAL:HG12	2:E:252:LEU:H	1.86	0.40
2:E:415:SER:HB2	2:E:459:MET:SD	2.61	0.40
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.51	0.40
1:A:438:ILE:O	1:A:442:VAL:HG13	2.22	0.40
1:B:129:VAL:HA	1:B:252:SER:OG	2.22	0.40
1:B:264:ALA:HB3	1:B:321:LEU:HD13	2.03	0.40
1:B:383:MET:HG2	1:B:438:ILE:HD11	2.02	0.40
2:D:384:LEU:O	2:D:385:GLN:C	2.65	0.40
2:E:147:ALA:HB2	2:E:357:ILE:CG2	2.51	0.40
2:F:309:ALA:C	2:F:310:ILE:HG13	2.45	0.40
2:F:366:GLU:O	2:F:370:VAL:HG23	2.21	0.40
1:A:268:TYR:O	1:A:270:ASP:HA	2.21	0.40
1:A:295:PRO:HD2	1:A:298:VAL:HB	2.02	0.40
1:B:47:VAL:HG13	1:B:90:ARG:HG2	2.03	0.40
1:B:55:PHE:O	1:B:56:SER:C	2.63	0.40
1:C:444:VAL:CG1	1:C:469:LEU:HD13	2.52	0.40
2:D:186:VAL:HG12	2:D:260:ARG:HB2	2.02	0.40
2:F:344:ILE:HG23	2:F:415:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	449 (93%)	33 (7%)	3 (1%)	21	38
1	B	475/510 (93%)	447 (94%)	25 (5%)	3 (1%)	21	38
1	C	490/510 (96%)	462 (94%)	26 (5%)	2 (0%)	30	49
2	D	465/482 (96%)	432 (93%)	26 (6%)	7 (2%)	8	16
2	E	464/482 (96%)	423 (91%)	35 (8%)	6 (1%)	9	18
2	F	464/482 (96%)	430 (93%)	31 (7%)	3 (1%)	21	38
3	G	116/272 (43%)	110 (95%)	4 (3%)	2 (2%)	7	13
All	All	2959/3248 (91%)	2753 (93%)	180 (6%)	26 (1%)	14	27

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	388	ILE
1	B	95	VAL
1	B	367	VAL
1	C	409	ASP
2	D	247	GLU
2	D	248	GLY
2	E	210	ASP
2	E	455	GLN
1	A	404	ALA
1	A	405	GLN
2	D	109	LYS
2	D	385	GLN
3	G	211	ASN
2	D	472	LYS
2	E	42	GLU
2	F	246	GLN
1	A	484	ARG

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Mol	Chain	Res	Type
1	B	452	TYR
2	D	246	GLN
2	D	448	GLU
2	F	455	GLN
2	E	156	GLY
3	G	81	ILE
2	F	420	VAL
2	E	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%)	367 (93%)	26 (7%)	15	32
1	B	388/412 (94%)	362 (93%)	26 (7%)	15	31
1	C	397/412 (96%)	368 (93%)	29 (7%)	13	27
2	D	377/386 (98%)	364 (97%)	13 (3%)	32	60
2	E	376/386 (97%)	355 (94%)	21 (6%)	19	39
2	F	376/386 (97%)	357 (95%)	19 (5%)	21	43
3	G	102/230 (44%)	96 (94%)	6 (6%)	18	37
All	All	2409/2624 (92%)	2269 (94%)	140 (6%)	18	38

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	59	LEU
1	A	87	ILE
1	A	99	VAL
1	A	102	GLU
1	A	121	ILE
1	A	136	ILE
1	A	141	SER
1	A	157	VAL

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Mol	Chain	Res	Type
1	A	175	LYS
1	A	211	SER
1	A	216	LEU
1	A	249	SER
1	A	286	ARG
1	A	301	LEU
1	A	338	ILE
1	A	344	SER
1	A	367	VAL
1	A	436	MET
1	A	449	VAL
1	A	459	SER
1	A	460	LYS
1	A	470	SER
1	A	472	VAL
1	A	479	LEU
1	A	505	LEU
1	B	28	THR
1	B	34	ILE
1	B	47	VAL
1	B	56	SER
1	B	59	LEU
1	B	102	GLU
1	B	123	SER
1	B	140	ILE
1	B	141	SER
1	B	151	LYS
1	B	157	VAL
1	B	159	ILE
1	B	211	SER
1	B	216	LEU
1	B	218	LYS
1	B	276	VAL
1	B	298	VAL
1	B	361	ILE
1	B	376	SER
1	B	380	THR
1	B	389	THR
1	B	422	VAL
1	B	434	SER
1	B	459	SER
1	B	479	LEU

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Mol	Chain	Res	Type
1	B	492	GLU
1	C	47	VAL
1	C	57	SER
1	C	59	LEU
1	C	64	LEU
1	C	74	VAL
1	C	87	ILE
1	C	91	THR
1	C	123	SER
1	C	132	LYS
1	C	140	ILE
1	C	165	GLU
1	C	188	ARG
1	C	193	THR
1	C	209	LYS
1	C	226	MET
1	C	262	LYS
1	C	298	VAL
1	C	307	GLU
1	C	334	VAL
1	C	391	LYS
1	C	414	THR
1	C	416	GLN
1	C	419	SER
1	C	438	ILE
1	C	444	VAL
1	C	449	VAL
1	C	459	SER
1	C	479	LEU
1	C	501	VAL
2	D	41	ARG
2	D	67	GLU
2	D	89	GLU
2	D	97	VAL
2	D	137	ILE
2	D	232	VAL
2	D	282	GLN
2	D	303	SER
2	D	335	LEU
2	D	358	MET
2	D	403	THR
2	D	420	VAL

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Mol	Chain	Res	Type
2	D	423	VAL
2	E	67	GLU
2	E	89	GLU
2	E	97	VAL
2	E	112	GLN
2	E	139	VAL
2	E	171	ASN
2	E	196	LEU
2	E	213	SER
2	E	215	VAL
2	E	223	ASN
2	E	232	VAL
2	E	251	VAL
2	E	279	VAL
2	E	282	GLN
2	E	293	GLN
2	E	297	THR
2	E	358	MET
2	E	395	GLU
2	E	420	VAL
2	E	431	LEU
2	E	444	ILE
2	F	9	THR
2	F	67	GLU
2	F	76	LEU
2	F	97	VAL
2	F	137	ILE
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	279	VAL
2	F	282	GLN
2	F	298	THR
2	F	303	SER
2	F	395	GLU
2	F	396	LEU
2	F	397	SER
2	F	455	GLN
3	G	20	THR

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Mol	Chain	Res	Type
3	G	78	CYS
3	G	84	SER
3	G	226	SER
3	G	240	SER
3	G	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	172	GLN
1	A	243	GLN
1	A	432	GLN
1	A	471	HIS
1	B	65	ASN
1	B	172	GLN
1	B	208	GLN
1	B	215	GLN
1	B	415	GLN
1	B	432	GLN
1	B	466	ASN
1	B	475	GLN
1	B	476	HIS
1	B	503	ASN
1	C	260	ASN
1	C	263	HIS
1	C	432	GLN
1	C	471	HIS
1	C	475	GLN
2	D	130	GLN
2	D	171	ASN
2	D	172	ASN
2	D	194	ASN
2	D	221	GLN
2	D	249	GLN
2	D	282	GLN
2	D	411	GLN
2	D	419	GLN
2	D	442	GLN
2	E	130	GLN
2	E	198	HIS
2	E	221	GLN

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Mol	Chain	Res	Type
2	E	223	ASN
2	E	263	GLN
2	E	282	GLN
2	E	293	GLN
2	E	379	GLN
2	E	385	GLN
2	E	442	GLN
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	361	ASN
2	F	367	HIS
2	F	419	GLN

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 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	$\# Z > 2$
7	AF3	D	602	9,5,6,1	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ANP	C	600	5	33,33,33	1.33	4 (12%)	45,52,52	1.11	3 (6%)
6	ADP	D	600	5,7	28,29,29	1.23	5 (17%)	43,45,45	0.81	1 (2%)
4	ANP	B	600	5	33,33,33	1.46	7 (21%)	45,52,52	1.10	1 (2%)
8	PO4	E	602	-	4,4,4	0.77	0	6,6,6	0.43	0
4	ANP	A	600	5	33,33,33	1.31	3 (9%)	45,52,52	0.97	1 (2%)
4	ANP	F	600	5	33,33,33	1.40	4 (12%)	45,52,52	1.05	5 (11%)

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	C	600	5	-	2/18/38/38	0/3/3/3
6	ADP	D	600	5,7	-	2/16/32/32	0/3/3/3
4	ANP	B	600	5	-	1/18/38/38	0/3/3/3
4	ANP	A	600	5	-	3/18/38/38	0/3/3/3
4	ANP	F	600	5	-	4/18/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	600	ANP	PG-O2G	-4.67	1.44	1.56
4	A	600	ANP	PG-O2G	-4.11	1.45	1.56
4	C	600	ANP	PG-O3G	-3.60	1.47	1.56
6	D	600	ADP	PA-O3A	3.53	1.63	1.59
4	B	600	ANP	PG-O2G	-3.41	1.47	1.56
4	F	600	ANP	PB-O2B	-3.29	1.48	1.56
4	C	600	ANP	PG-O2G	-3.28	1.48	1.56
4	F	600	ANP	PA-O3A	-3.28	1.56	1.59
4	B	600	ANP	PB-O2B	-3.27	1.48	1.56
4	A	600	ANP	PG-O3G	-3.23	1.48	1.56
4	C	600	ANP	PB-O2B	-3.16	1.48	1.56
4	A	600	ANP	PB-O2B	-3.14	1.48	1.56
4	B	600	ANP	PG-O3G	-2.93	1.49	1.56
4	B	600	ANP	PB-O3A	2.83	1.62	1.59
6	D	600	ADP	PB-O2B	-2.49	1.45	1.54
6	D	600	ADP	PB-O3B	-2.46	1.45	1.54
4	B	600	ANP	PA-O3A	2.30	1.62	1.59
4	B	600	ANP	C2-N3	-2.22	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	600	ANP	PB-O1B	2.16	1.49	1.46
4	B	600	ANP	C2-N1	2.05	1.37	1.33
4	C	600	ANP	PA-O2A	-2.05	1.45	1.55
6	D	600	ADP	C2-N1	2.04	1.37	1.33
6	D	600	ADP	C2-N3	-2.03	1.30	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	ANP	O1B-PB-N3B	4.85	118.91	111.77
4	A	600	ANP	O1G-PG-N3B	-3.57	106.51	111.77
4	C	600	ANP	O1G-PG-N3B	-3.20	107.05	111.77
4	F	600	ANP	O1G-PG-N3B	-2.77	107.69	111.77
6	D	600	ADP	O2B-PB-O3A	2.52	113.10	104.64
4	C	600	ANP	C2'-C3'-C4'	2.20	106.86	102.61
4	F	600	ANP	O2B-PB-O3A	2.17	111.87	104.64
4	F	600	ANP	C1'-N9-C8	2.12	131.80	127.09
4	C	600	ANP	O2A-PA-O5'	2.03	116.77	107.57
4	F	600	ANP	O2G-PG-O3G	2.02	113.02	107.59
4	F	600	ANP	O3A-PA-O1A	2.02	116.77	110.70

There are no chirality outliers.

All (12) torsion outliers are listed below:

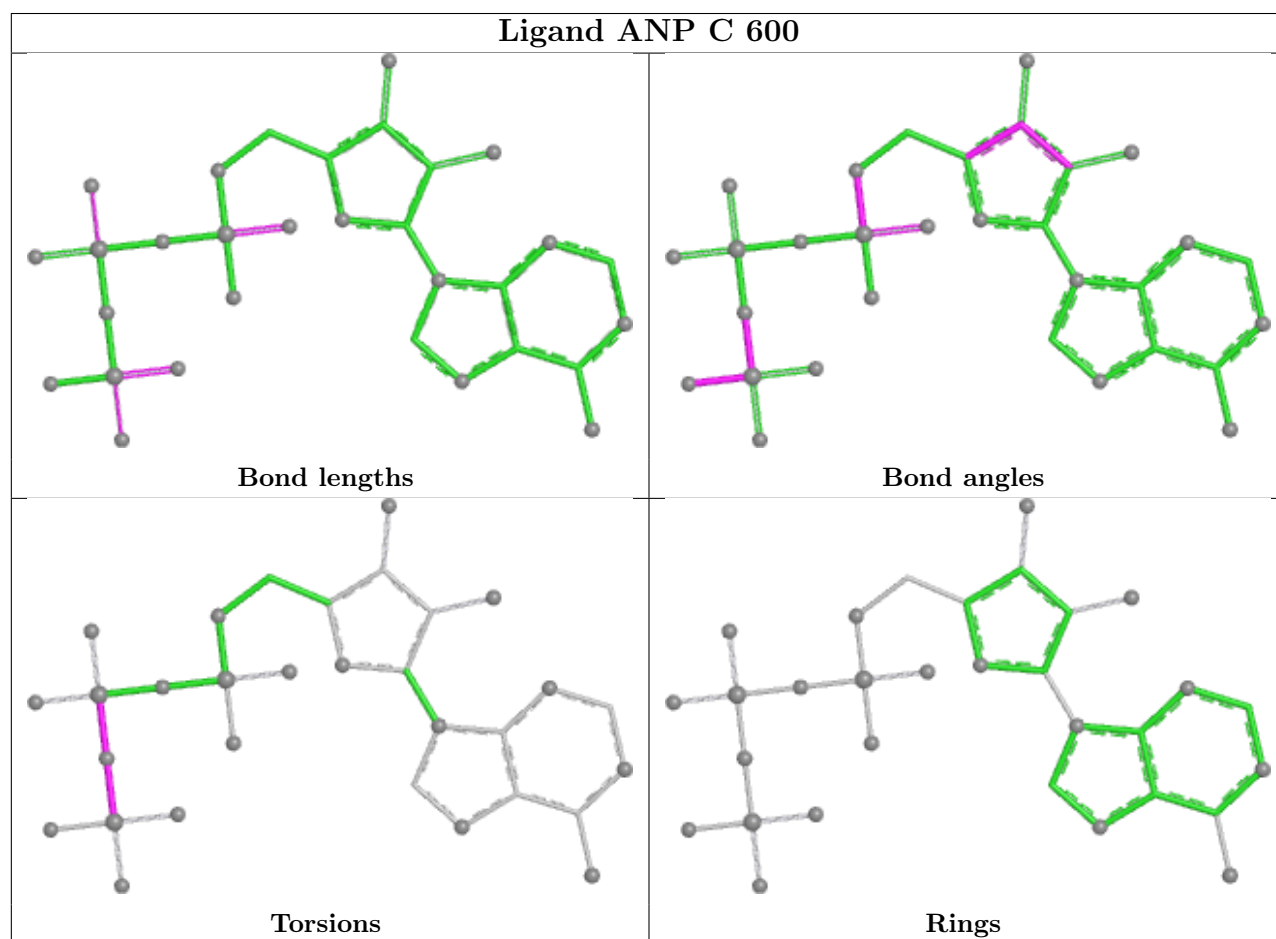
Mol	Chain	Res	Type	Atoms
4	A	600	ANP	PB-N3B-PG-O1G
4	A	600	ANP	PG-N3B-PB-O1B
4	B	600	ANP	PG-N3B-PB-O1B
4	C	600	ANP	PB-N3B-PG-O1G
4	C	600	ANP	PG-N3B-PB-O1B
4	F	600	ANP	PB-N3B-PG-O1G
4	F	600	ANP	PG-N3B-PB-O1B
4	F	600	ANP	PA-O3A-PB-O2B
6	D	600	ADP	PA-O3A-PB-O2B
6	D	600	ADP	PA-O3A-PB-O3B
4	F	600	ANP	PA-O3A-PB-O1B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

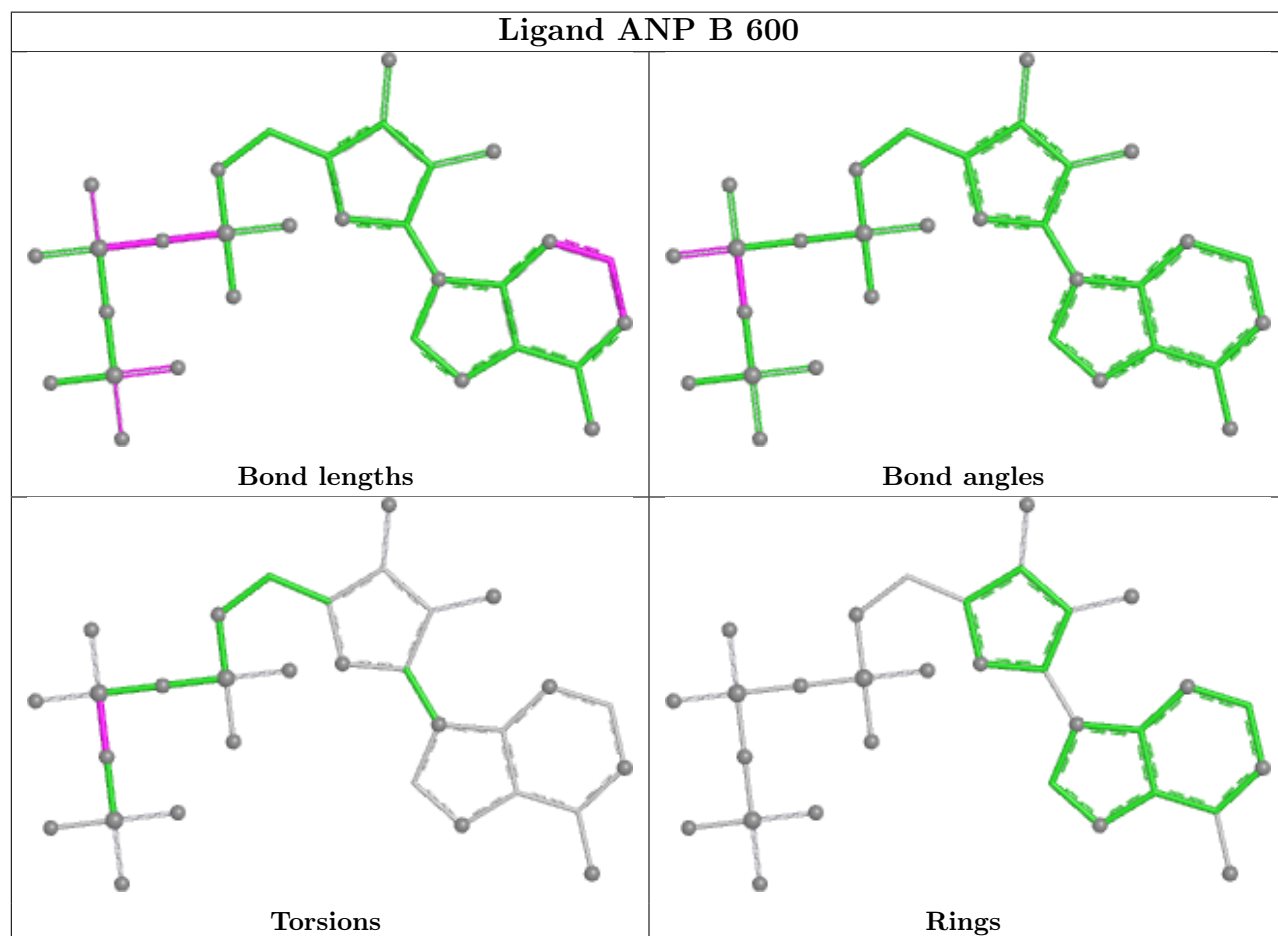
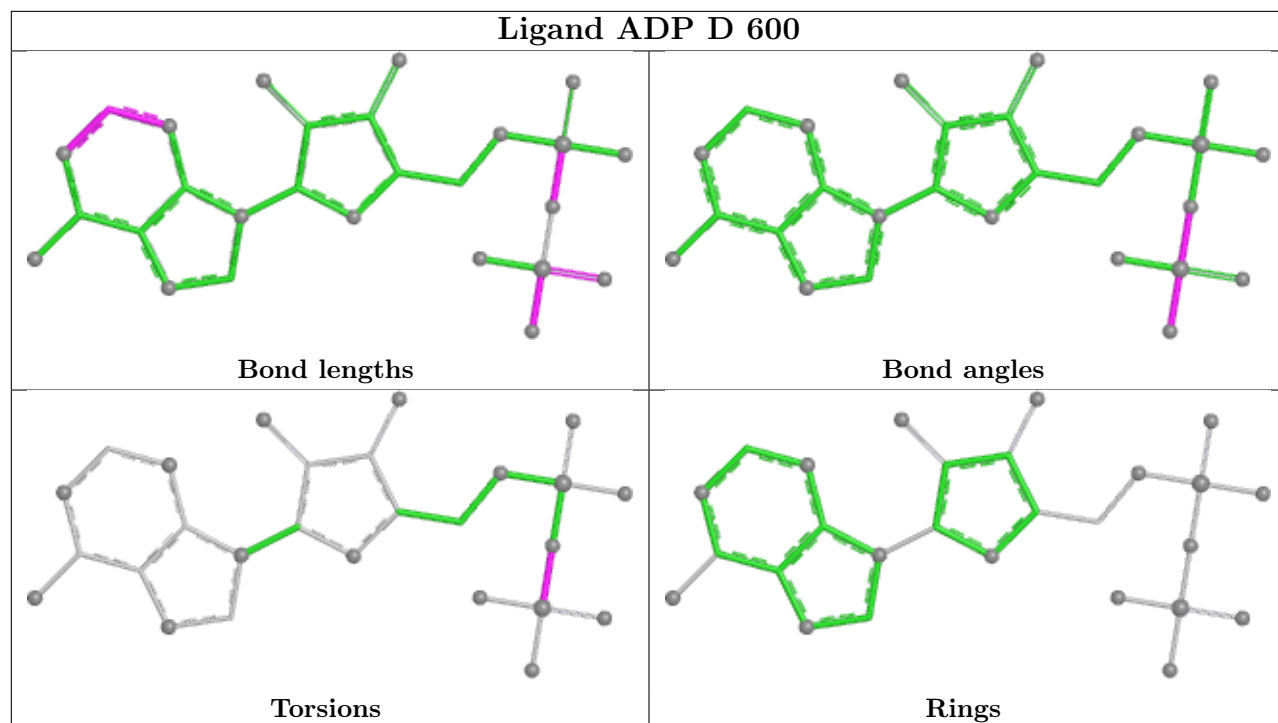
There are no ring outliers.

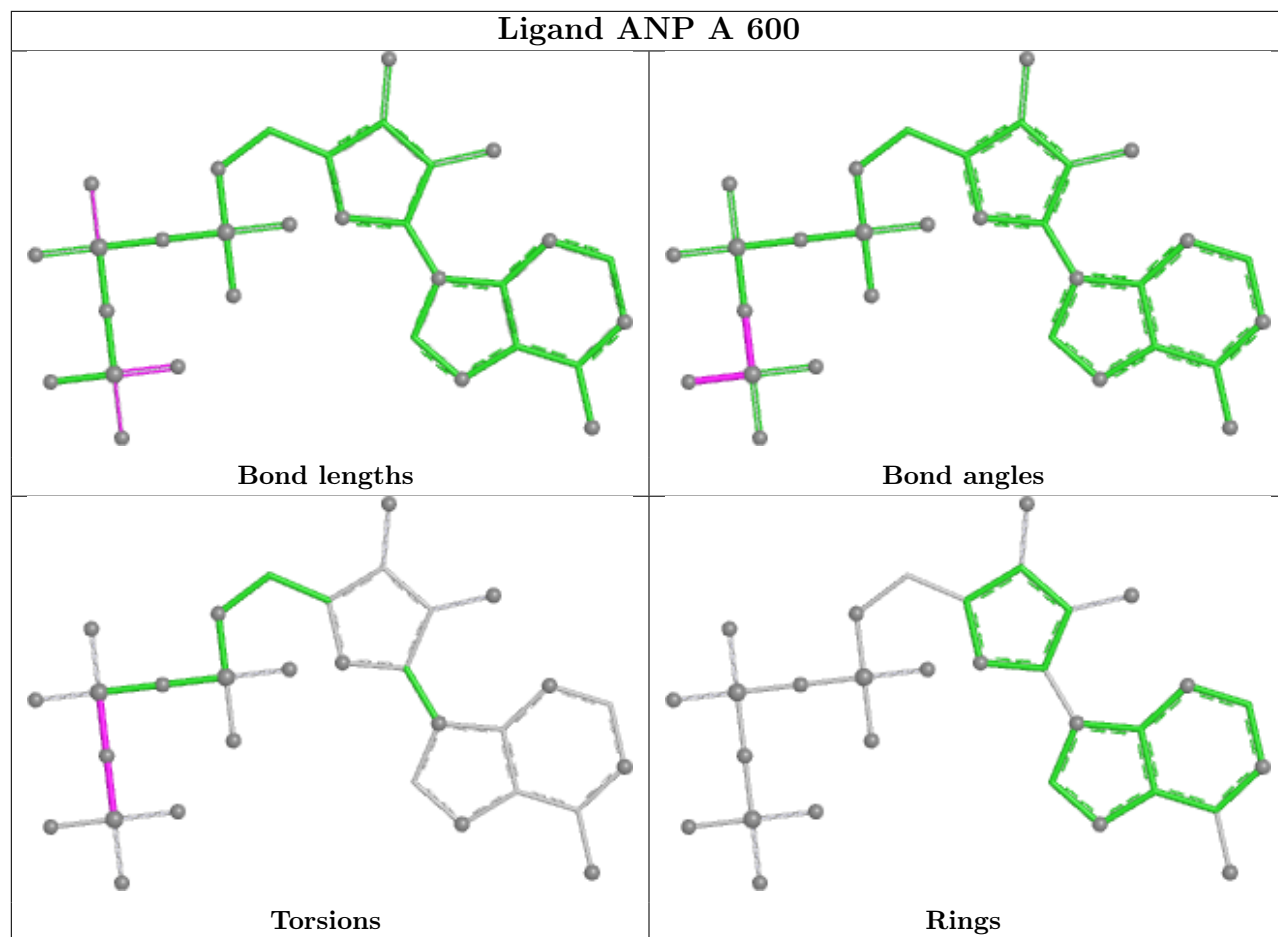
5 monomers are involved in 8 short contacts:

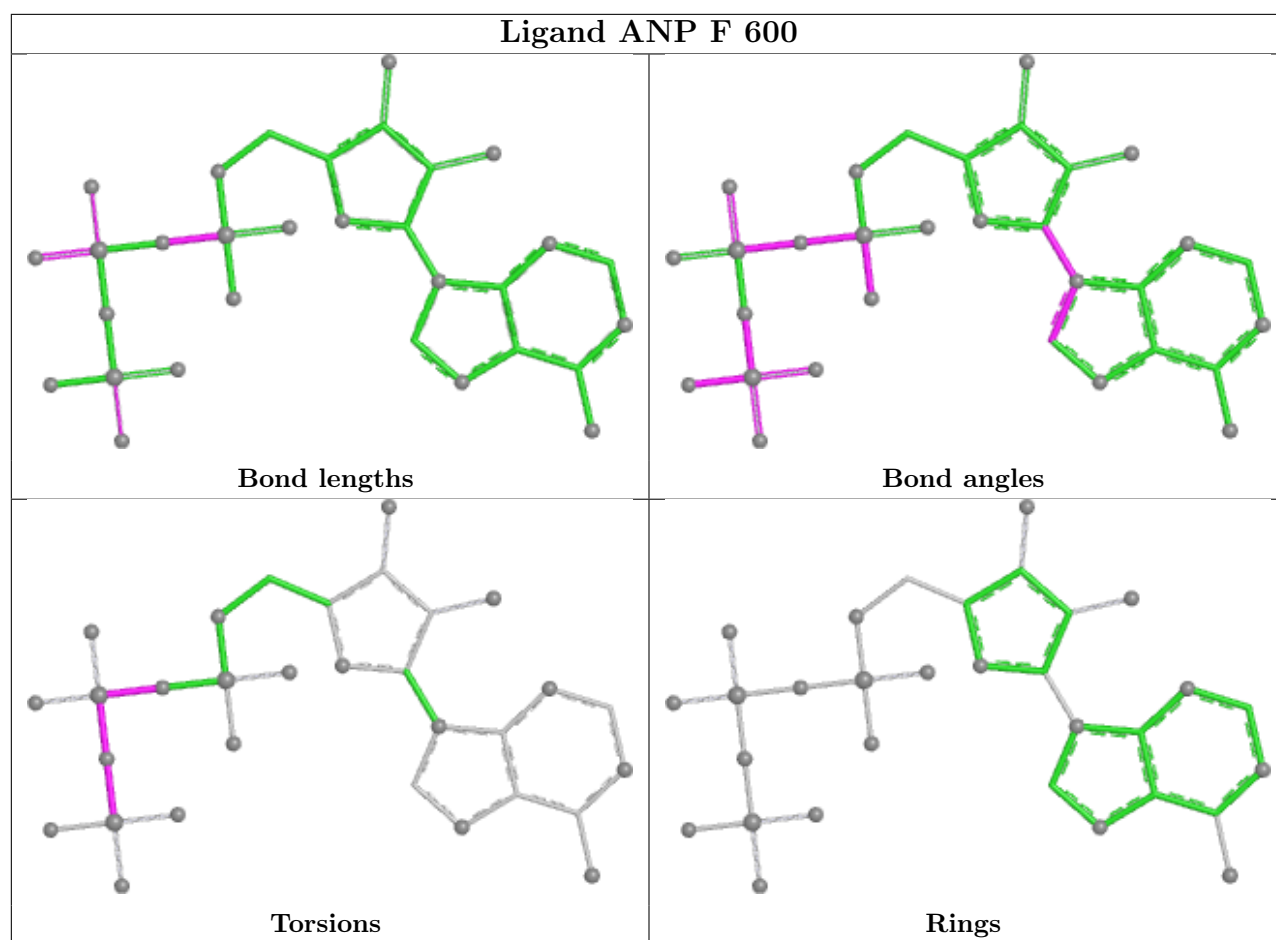
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	602	AF3	1	0
4	C	600	ANP	1	0
6	D	600	ADP	1	0
4	B	600	ANP	4	0
4	F	600	ANP	1	0

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%)	0.11	21 (4%) 40 35	26, 46, 76, 110	0
1	B	479/510 (93%)	0.33	34 (7%) 22 19	25, 43, 97, 110	0
1	C	492/510 (96%)	-0.12	9 (1%) 67 64	24, 38, 65, 106	0
2	D	467/482 (96%)	-0.04	14 (2%) 52 48	24, 40, 73, 103	0
2	E	466/482 (96%)	0.51	34 (7%) 21 19	26, 51, 102, 119	0
2	F	466/482 (96%)	-0.03	11 (2%) 59 55	24, 41, 72, 90	0
3	G	122/272 (44%)	1.12	32 (26%) 1 1	29, 68, 108, 111	0
All	All	2979/3248 (91%)	0.17	155 (5%) 33 29	24, 44, 88, 119	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	510	ALA	7.4
1	B	410	LEU	6.2
2	E	390	ILE	5.7
3	G	44	TYR	5.5
2	D	9	THR	5.3
2	F	474	ALA	5.1
2	E	423	VAL	5.1
2	E	389	ALA	4.9
3	G	1	ALA	4.8
2	E	28	GLY	4.7
1	B	416	GLN	4.7
1	B	358	TYR	4.7
1	C	408	SER	4.6
2	D	474	ALA	4.6
1	A	93	ALA	4.5
3	G	209	LEU	4.5
2	F	248	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
3	G	43	VAL	4.2
1	B	401	ALA	4.2
3	G	214	TYR	4.1
2	E	424	PHE	3.9
2	E	388	ILE	3.9
1	B	496	LYS	3.9
1	A	91	THR	3.9
3	G	85	VAL	3.8
2	E	420	VAL	3.7
3	G	90	LYS	3.7
1	C	407	GLY	3.7
3	G	89	MET	3.6
2	E	393	MET	3.5
2	D	249	GLN	3.5
2	E	474	ALA	3.5
1	A	412	ALA	3.4
1	C	506	ALA	3.3
2	E	456	ALA	3.3
1	C	409	ASP	3.3
3	G	33	ARG	3.3
2	E	387	ILE	3.3
3	G	40	PRO	3.2
2	F	249	GLN	3.1
1	B	505	LEU	3.1
2	E	391	LEU	3.0
1	B	458	PRO	3.0
3	G	215	TYR	2.9
1	A	408	SER	2.9
3	G	86	ALA	2.9
3	G	213	ILE	2.9
3	G	78	CYS	2.9
2	E	403	THR	2.9
1	B	395	ALA	2.9
1	B	392	LEU	2.9
1	C	410	LEU	2.9
2	D	248	GLY	2.9
3	G	35	GLU	2.8
3	G	218	LYS	2.8
1	A	94	ILE	2.8
2	E	419	GLN	2.8
2	E	421	ALA	2.7
3	G	221	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	357	PHE	2.7
1	B	487	GLY	2.7
1	B	412	ALA	2.7
3	G	80	ALA	2.7
1	A	92	GLY	2.7
3	G	212	ILE	2.6
3	G	36	ARG	2.6
1	B	474	SER	2.6
1	B	397	TYR	2.6
1	B	400	VAL	2.6
2	E	344	ILE	2.6
1	A	414	THR	2.6
2	F	9	THR	2.6
2	F	175	LYS	2.6
3	G	39	LYS	2.6
2	F	395	GLU	2.5
2	D	473	LEU	2.5
3	G	217	LEU	2.5
3	G	34	ALA	2.5
1	A	499	GLU	2.5
1	B	422	VAL	2.5
2	D	110	THR	2.5
2	E	9	THR	2.5
1	B	413	ALA	2.5
2	D	27	GLU	2.5
2	D	178	GLY	2.5
2	E	157	GLY	2.5
1	A	409	ASP	2.5
2	E	402	LEU	2.5
1	B	495	ALA	2.5
3	G	25	MET	2.5
2	D	247	GLU	2.4
2	E	455	GLN	2.4
2	E	401	LYS	2.4
2	E	472	LYS	2.4
1	A	410	LEU	2.4
1	B	418	LEU	2.4
1	C	405	GLN	2.4
3	G	211	ASN	2.4
1	B	387	ALA	2.4
1	C	195	GLU	2.4
2	E	395	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	403	PHE	2.4
3	G	210	ALA	2.4
1	C	414	THR	2.4
3	G	84	SER	2.4
2	F	246	GLN	2.4
1	B	388	GLY	2.3
2	D	28	GLY	2.3
2	E	215	VAL	2.3
1	B	459	SER	2.3
1	A	487	GLY	2.3
1	B	452	TYR	2.3
1	A	407	GLY	2.3
1	A	510	ALA	2.3
1	C	406	PHE	2.3
1	A	143	ARG	2.3
1	B	484	ARG	2.3
3	G	79	GLY	2.2
2	D	396	LEU	2.2
2	D	10	THR	2.2
2	E	384	LEU	2.2
1	A	121	ILE	2.2
3	G	37	GLU	2.2
2	E	461	GLY	2.2
1	B	492	GLU	2.2
1	A	197	LYS	2.2
1	A	402	ALA	2.1
2	F	473	LEU	2.1
3	G	77	LEU	2.1
1	B	457	GLU	2.1
2	E	210	ASP	2.1
1	B	501	VAL	2.1
1	B	415	GLN	2.1
2	F	270	ALA	2.1
2	F	178	GLY	2.1
2	F	447	GLY	2.1
1	A	381	ARG	2.1
2	D	390	ILE	2.1
2	E	467	VAL	2.1
2	E	473	LEU	2.1
1	A	482	LYS	2.1
1	B	196	LYS	2.1
1	B	488	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	36	ASP	2.1
2	E	470	ALA	2.0
1	B	394	LEU	2.0
2	E	76	LEU	2.0
2	D	475	GLU	2.0
2	E	109	LYS	2.0
1	A	411	ASP	2.0
2	E	180	TYR	2.0
2	E	449	TYR	2.0
1	B	479	LEU	2.0
3	G	87	LYS	2.0
3	G	83	SER	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.

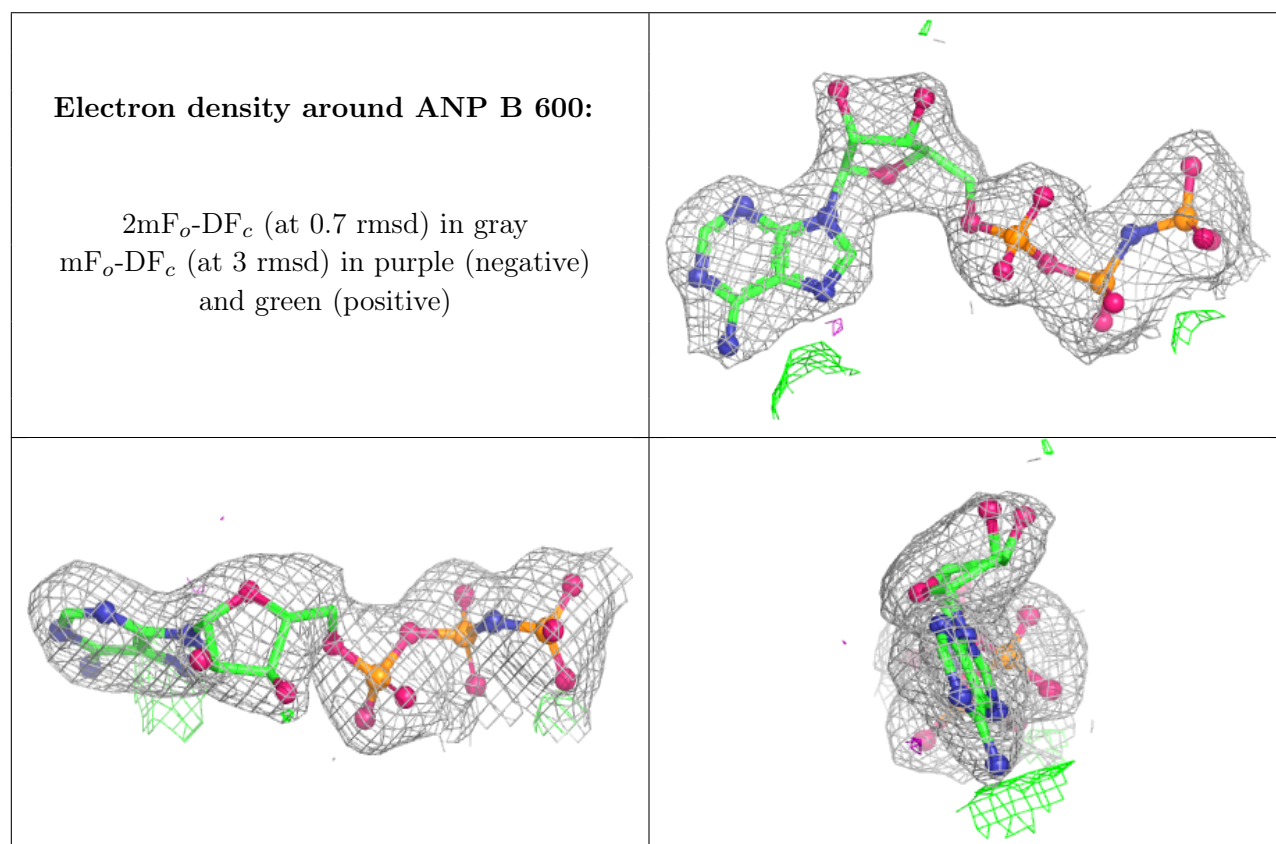
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	PO4	E	602	5/5	0.70	0.18	86,87,87,87	0
5	MG	A	601	1/1	0.88	0.09	41,41,41,41	0
7	AF3	D	602	4/4	0.90	0.22	41,41,43,45	0
5	MG	B	601	1/1	0.95	0.04	37,37,37,37	0
5	MG	F	601	1/1	0.97	0.09	32,32,32,32	0
4	ANP	B	600	31/31	0.97	0.07	32,47,51,54	0
4	ANP	C	600	31/31	0.97	0.07	29,37,41,45	0
6	ADP	D	600	27/27	0.98	0.06	28,33,35,36	0
4	ANP	F	600	31/31	0.98	0.07	34,38,45,45	0
4	ANP	A	600	31/31	0.98	0.06	29,36,40,42	0
5	MG	C	601	1/1	0.99	0.03	28,28,28,28	0

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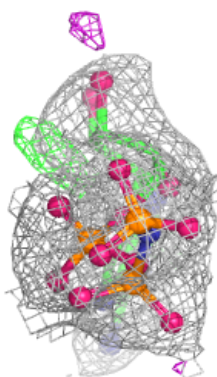
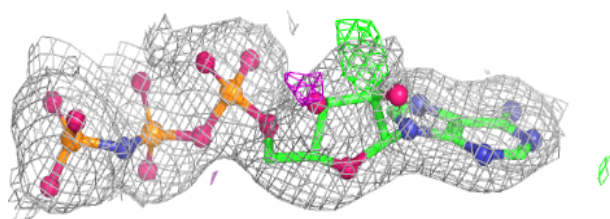
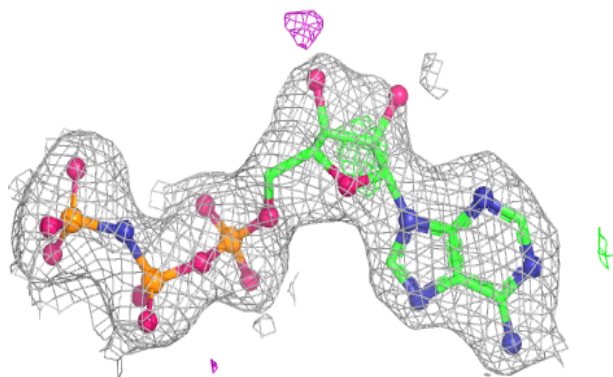
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	D	601	1/1	0.99	0.06	33,33,33,33	0

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.

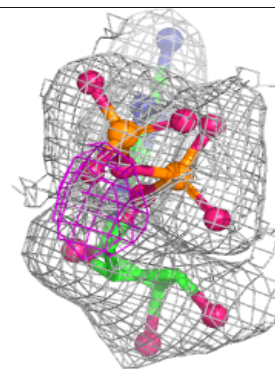
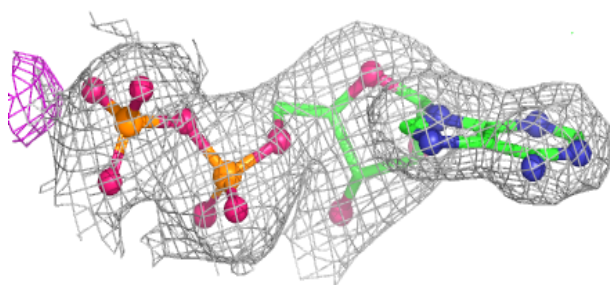
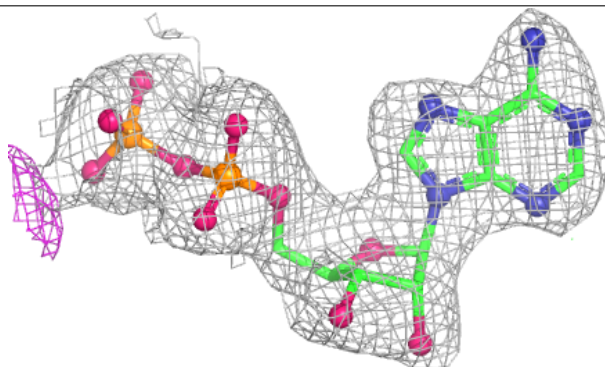


Electron density around ANP C 600:

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

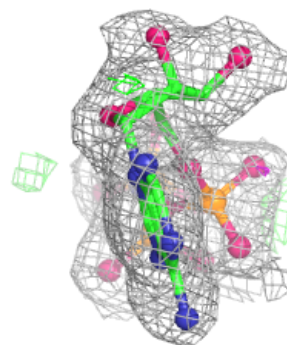
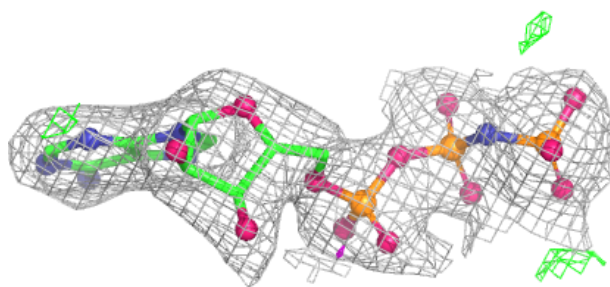
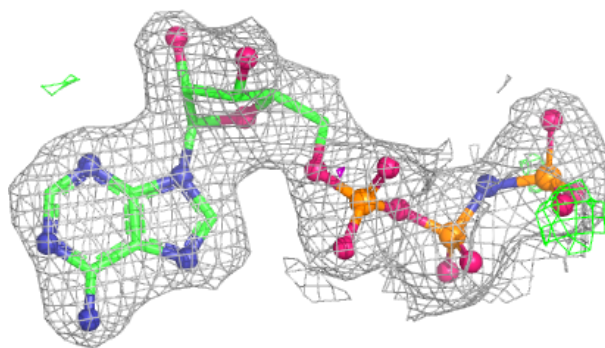
**Electron density around ADP D 600:**

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

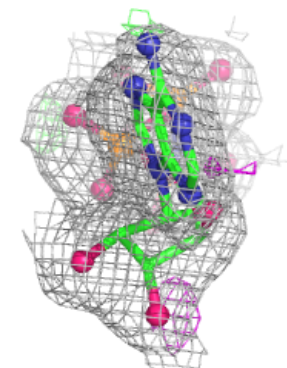
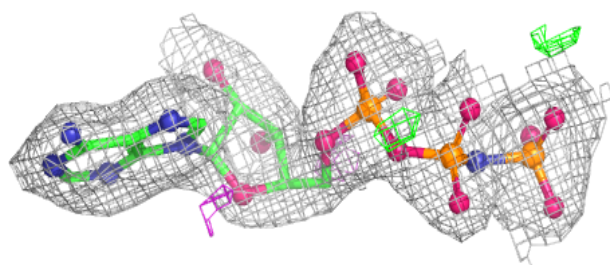
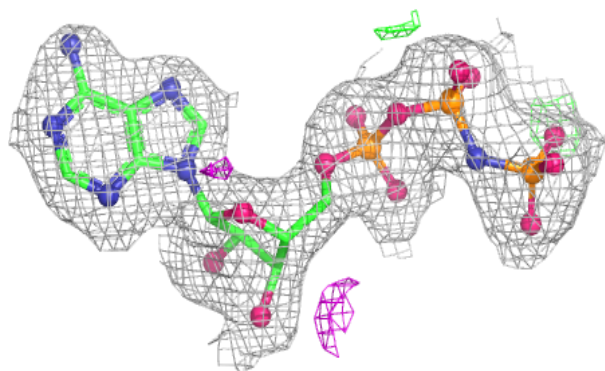


Electron density around ANP F 600:

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

**Electron density around ANP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.