



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:06 AM UTC

PDB ID : 1H8E / pdb_00001h8e
Title : (ADP.AIF4)2(ADP.SO4) bovine F1-ATPase (all three catalytic sites occupied)
Authors : Menz, R.I.; Walker, J.E.; Leslie, A.G.W.
Deposited on : 2001-02-02
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 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

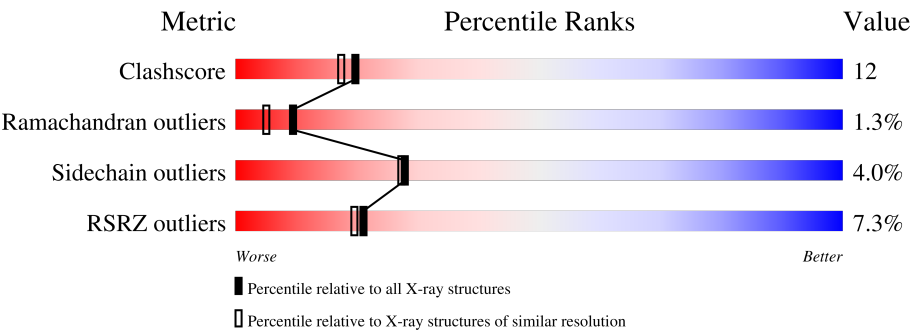
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	79%14%5%
1	B	510	73%18%6%
1	C	510	76%18%. .
2	D	482	76%18%. .
2	E	482	14%61%28%6%
2	F	482	3%76%17%. .

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Mol	Chain	Length	Quality of chain
3	G	272	
4	H	146	
5	I	50	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	ALF	D	620	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 26329 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	486	Total	C	N	O	S	0	0	0
			3705	2334	654	705	12			
1	B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	C	488	Total	C	N	O	S	0	0	0
			3718	2341	656	709	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	454	Total	C	N	O	S	0	0	0
			3447	2186	586	664	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	244	Total	C	N	O	S	0	0	0
			1891	1191	328	364	8			

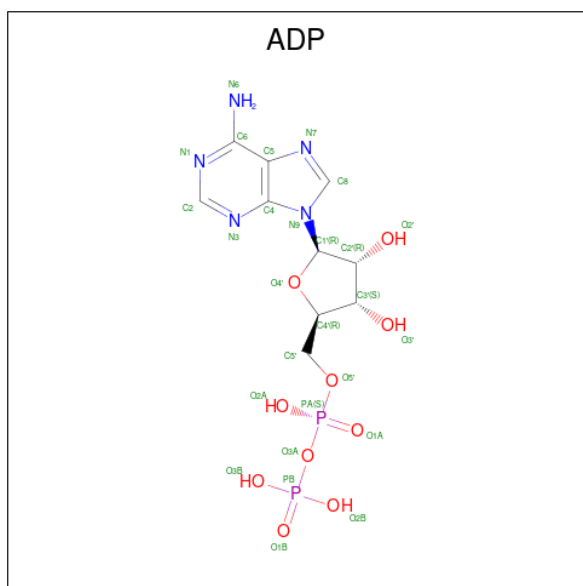
- Molecule 4 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	89	Total	C	N	O	S	0	0	0
			662	420	109	131	2			

- Molecule 5 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	36	Total	C	N	O	S	0	0	0
			281	180	51	49	1			

- 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	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

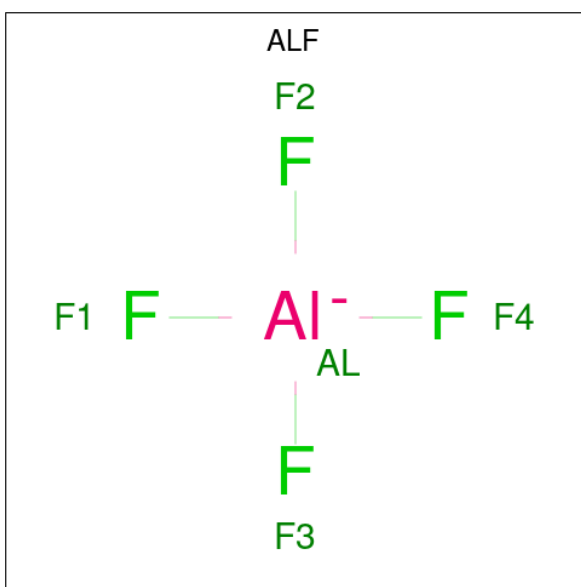
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	E	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



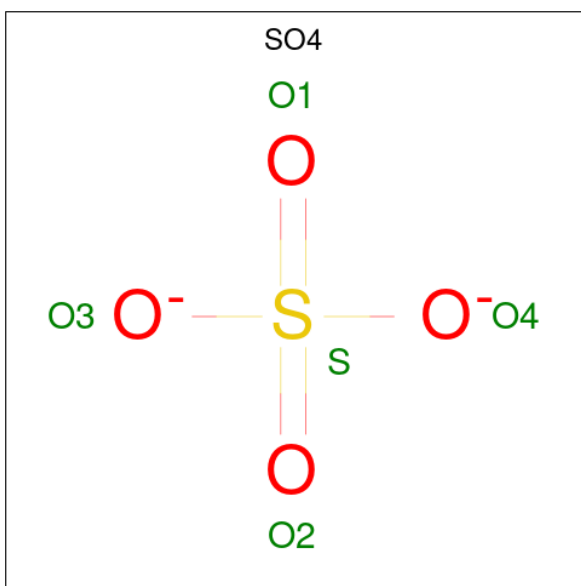
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

- Molecule 9 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	Al	F	0	0
			5	1	4		
9	F	1	Total	Al	F	0	0
			5	1	4		

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	O	S	0	0
			5	4	1		

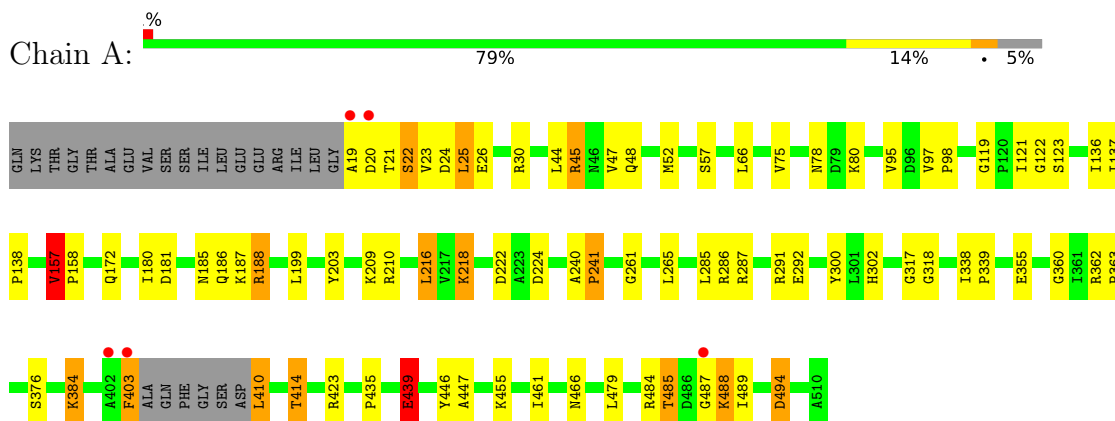
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	310	Total 310	O 310	0	0
11	B	241	Total 241	O 241	0	0
11	C	322	Total 322	O 322	0	0
11	D	310	Total 310	O 310	0	0
11	E	181	Total 181	O 181	0	0
11	F	286	Total 286	O 286	0	0
11	G	39	Total 39	O 39	0	0
11	H	3	Total 3	O 3	0	0
11	I	1	Total 1	O 1	0	0

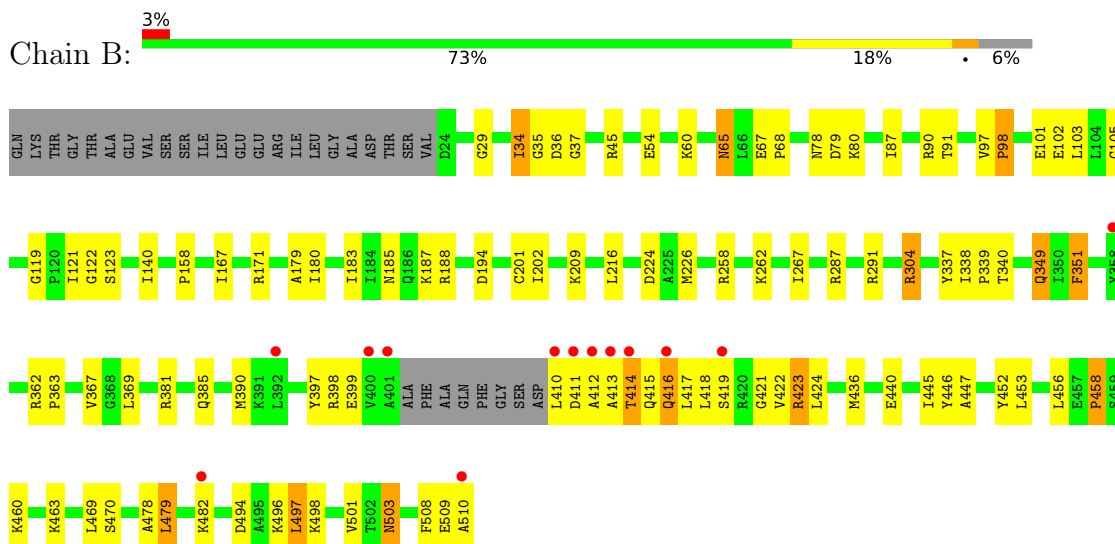
3 Residue-property plots [i](#)

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

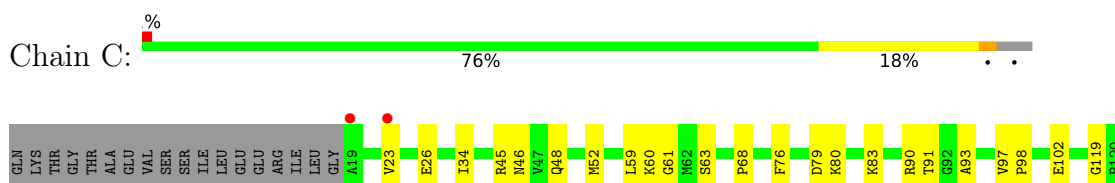
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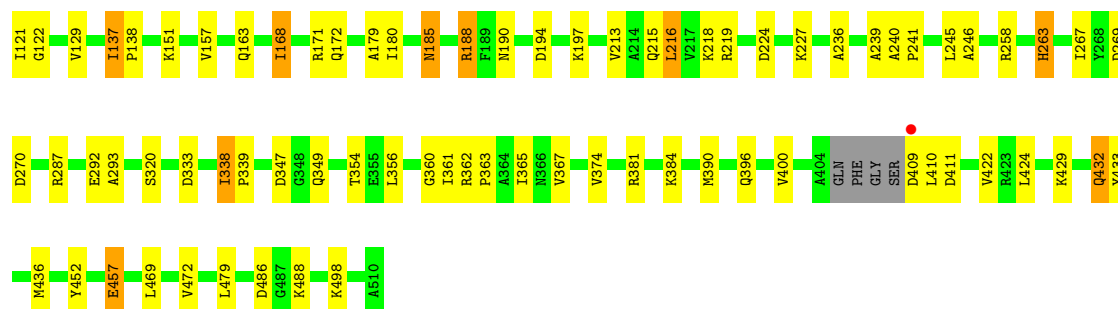


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

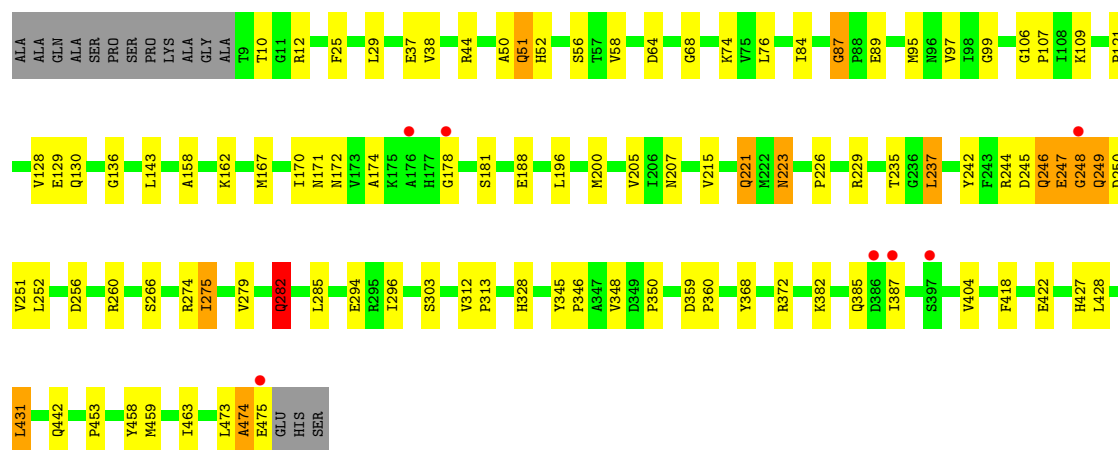
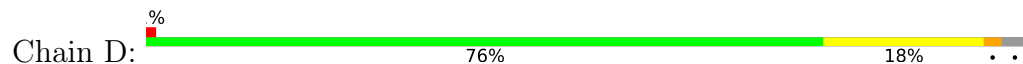


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

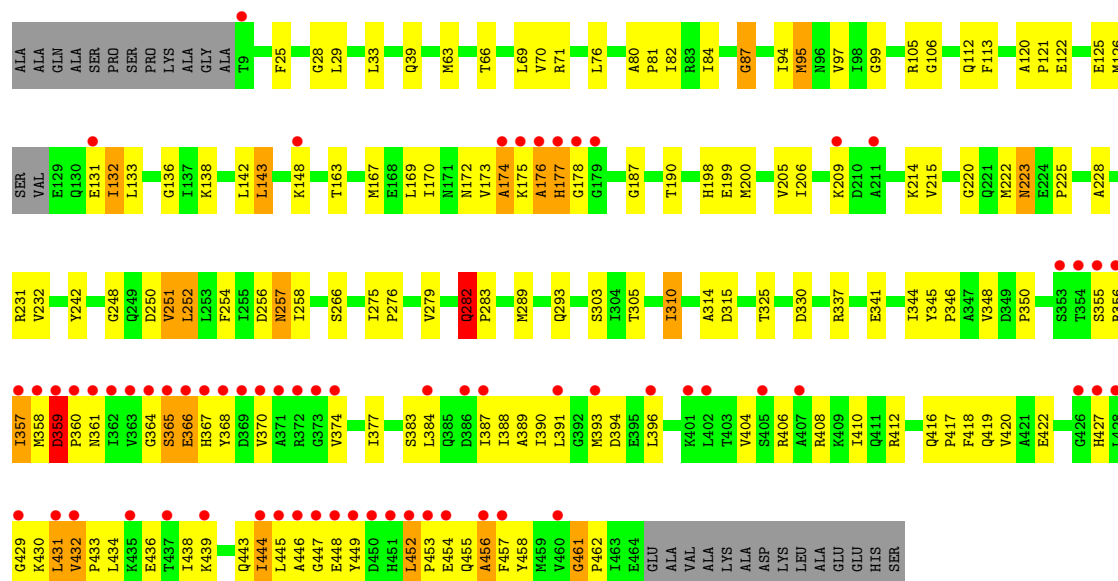




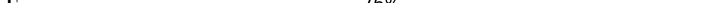
• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

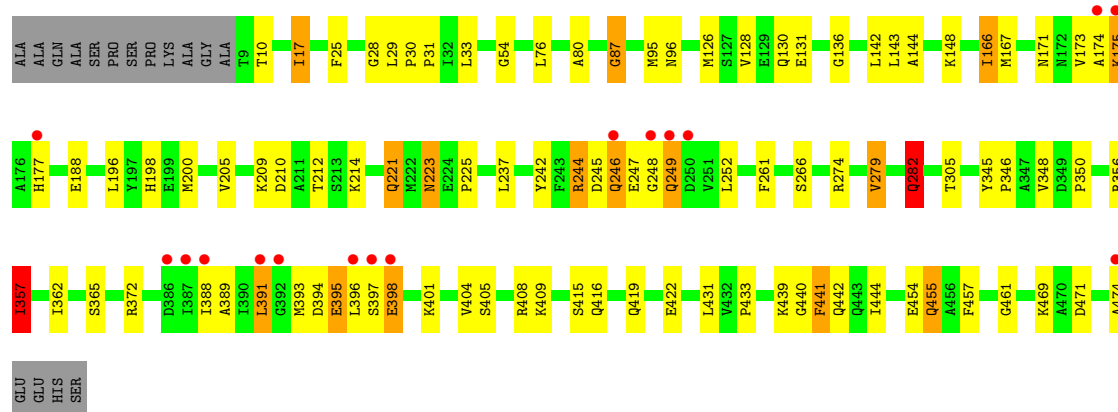


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

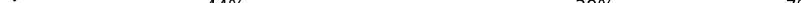


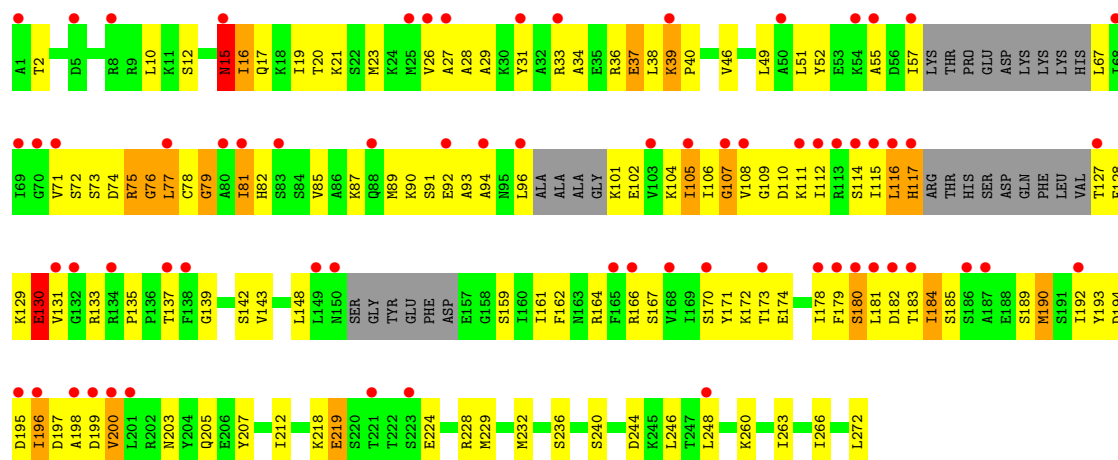
• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

Chain F:  3% 76% 17% . .



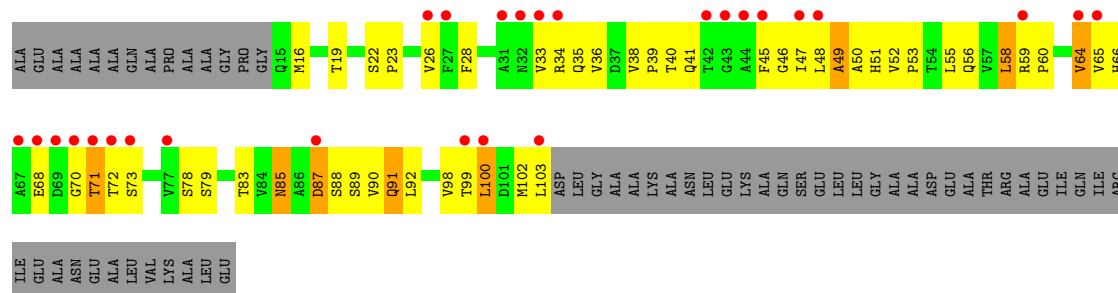
- Molecule 3: BOVINE MITOCHONDRIAL F1-ATPASE

Chain G: 

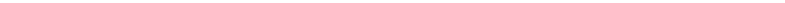


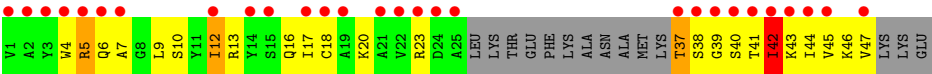
- Molecule 4: BOVINE MITOCHONDRIAL F1-ATPASE

Chain H: 



- Molecule 5: BOVINE MITOCHONDRIAL F1-ATPASE

Chain I:  56% 24% 40% 6% 28%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	267.70Å 106.20Å 138.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	13.50 – 2.00 13.50 – 2.00	Depositor EDS
% Data completeness (in resolution range)	79.6 (13.50-2.00) 79.2 (13.50-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.264 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26329	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 2.79% 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: ADP, MG, ALF, GOL, SO4

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	0.83	1/3754 (0.0%)	1.56	36/5064 (0.7%)
1	B	0.81	0/3704	1.48	21/4995 (0.4%)
1	C	0.88	0/3767	1.56	31/5082 (0.6%)
2	D	0.87	0/3596	1.58	43/4879 (0.9%)
2	E	0.76	0/3503	1.48	33/4752 (0.7%)
2	F	0.84	0/3587	1.55	32/4867 (0.7%)
3	G	0.68	1/1907 (0.1%)	1.47	20/2556 (0.8%)
4	H	0.56	0/674	1.34	5/922 (0.5%)
5	I	0.63	0/284	1.42	3/381 (0.8%)
All	All	0.81	2/24776 (0.0%)	1.53	224/33498 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	76	GLY	N-CA	-6.79	1.35	1.45
1	A	122	GLY	N-CA	6.18	1.54	1.45

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	250	ASP	CA-CB-CG	12.19	124.79	112.60
1	B	351	PHE	CA-CB-CG	11.83	125.63	113.80
2	F	198	HIS	CA-CB-CG	-11.81	101.99	113.80
1	A	188	ARG	CD-NE-CZ	10.24	138.74	124.40
3	G	75	ARG	CA-C-N	9.52	140.06	121.41
3	G	75	ARG	C-N-CA	9.52	140.06	121.41
2	E	432	VAL	N-CA-C	9.51	116.96	107.55
1	C	188	ARG	NE-CZ-NH2	9.16	127.44	119.20
2	E	105	ARG	CD-NE-CZ	8.92	136.88	124.40
2	D	229	ARG	CD-NE-CZ	8.87	136.82	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	15	ASN	CA-CB-CG	8.43	121.03	112.60
1	C	486	ASP	CA-CB-CG	8.30	120.90	112.60
2	E	282	GLN	CA-C-N	8.15	128.25	119.28
2	E	282	GLN	C-N-CA	8.15	128.25	119.28
2	D	12	ARG	CD-NE-CZ	7.94	135.52	124.40
1	C	188	ARG	NE-CZ-NH1	-7.83	113.67	121.50
2	F	391	LEU	N-CA-C	7.80	121.24	112.97
1	B	258	ARG	CD-NE-CZ	7.65	135.11	124.40
2	E	432	VAL	CA-C-O	7.51	124.95	119.25
1	C	258	ARG	CD-NE-CZ	7.49	134.88	124.40
2	D	274	ARG	CA-C-N	7.46	131.52	121.23
2	D	274	ARG	C-N-CA	7.46	131.52	121.23
1	A	45	ARG	CD-NE-CZ	7.42	134.79	124.40
1	A	78	ASN	CA-CB-CG	7.33	119.93	112.60
2	D	249	GLN	N-CA-C	7.31	121.75	110.42
1	C	91	THR	N-CA-C	-7.25	104.69	113.97
2	D	418	PHE	CA-CB-CG	7.23	121.03	113.80
1	A	265	LEU	CA-C-N	-7.17	113.16	123.06
1	A	265	LEU	C-N-CA	-7.17	113.16	123.06
1	B	349	GLN	CB-CG-CD	7.16	124.78	112.60
3	G	117	HIS	CA-CB-CG	-7.16	106.64	113.80
1	A	24	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	66	LEU	CA-C-O	-7.00	113.26	120.54
2	D	442	GLN	CA-CB-CG	6.99	128.08	114.10
1	C	157	VAL	CA-C-N	6.98	126.95	119.76
1	C	157	VAL	C-N-CA	6.98	126.95	119.76
2	F	274	ARG	CA-CB-CG	6.80	127.70	114.10
1	C	411	ASP	CA-CB-CG	6.77	119.37	112.60
4	H	45	PHE	N-CA-C	6.74	120.50	109.72
2	E	94	ILE	N-CA-CB	6.70	120.36	111.25
2	E	198	HIS	CA-CB-CG	-6.69	107.11	113.80
1	A	439	GLU	CA-CB-CG	6.61	127.32	114.10
1	A	121	ILE	CA-C-O	-6.59	113.34	120.85
3	G	135	PRO	CA-C-N	6.39	126.36	120.03
3	G	135	PRO	C-N-CA	6.39	126.36	120.03
2	E	359	ASP	CA-CB-CG	6.38	118.98	112.60
1	B	167	ILE	N-CA-CB	6.36	119.69	111.67
2	D	121	PRO	N-CA-CB	6.36	108.84	103.25
1	C	263	HIS	CA-CB-CG	-6.34	107.46	113.80
1	B	90	ARG	CD-NE-CZ	6.34	133.27	124.40
1	A	172	GLN	OE1-CD-NE2	-6.33	116.27	122.60
2	E	225	PRO	CA-C-N	6.33	126.08	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	225	PRO	C-N-CA	6.33	126.08	119.05
1	A	285	LEU	CA-C-O	6.29	126.89	119.28
2	E	432	VAL	CA-C-N	6.15	126.09	119.76
2	E	432	VAL	C-N-CA	6.15	126.09	119.76
2	D	178	GLY	N-CA-C	-6.14	101.55	112.54
1	A	302	HIS	CA-CB-CG	-6.13	107.67	113.80
2	D	256	ASP	CA-C-N	6.13	132.74	121.70
2	D	256	ASP	C-N-CA	6.13	132.74	121.70
2	D	143	LEU	N-CA-C	6.13	119.95	112.23
2	E	225	PRO	N-CA-CB	6.10	109.00	103.08
2	F	282	GLN	CA-C-N	6.10	125.78	119.56
2	F	282	GLN	C-N-CA	6.10	125.78	119.56
2	E	257	ASN	CA-CB-CG	6.09	118.69	112.60
1	C	90	ARG	CD-NE-CZ	6.08	132.91	124.40
2	F	143	LEU	N-CA-C	6.08	120.90	112.45
1	A	121	ILE	N-CA-C	-6.08	100.87	108.89
1	A	287	ARG	CA-C-N	6.06	126.62	120.38
1	A	287	ARG	C-N-CA	6.06	126.62	120.38
1	A	300	TYR	CA-CB-CG	6.06	124.80	113.90
1	A	181	ASP	CA-CB-CG	-6.02	106.58	112.60
2	E	283	PRO	N-CA-CB	6.00	109.87	103.39
1	C	365	ILE	N-CA-C	5.97	117.38	108.54
1	C	374	VAL	CA-C-O	5.96	124.30	119.29
1	A	157	VAL	CA-C-N	5.96	125.89	119.76
1	A	157	VAL	C-N-CA	5.96	125.89	119.76
2	D	171	ASN	CA-CB-CG	5.92	118.52	112.60
3	G	107	GLY	CA-C-O	-5.91	116.33	120.94
1	C	190	ASN	CA-CB-CG	-5.90	106.70	112.60
2	E	71	ARG	CD-NE-CZ	5.90	132.65	124.40
2	D	282	GLN	OE1-CD-NE2	-5.88	116.72	122.60
3	G	200	VAL	CA-C-O	5.88	127.14	119.85
2	D	372	ARG	CD-NE-CZ	5.87	132.62	124.40
1	C	432	GLN	OE1-CD-NE2	5.87	128.47	122.60
1	B	304	ARG	NE-CZ-NH1	-5.86	115.64	121.50
4	H	85	ASN	CA-CB-CG	-5.85	106.75	112.60
1	B	494	ASP	CA-CB-CG	5.84	118.44	112.60
2	D	252	LEU	CA-C-O	-5.82	114.09	120.43
2	E	293	GLN	OE1-CD-NE2	-5.79	116.81	122.60
3	G	15	ASN	OD1-CG-ND2	-5.79	116.81	122.60
2	E	303	SER	N-CA-C	5.79	117.86	109.07
2	F	173	VAL	N-CA-CB	-5.78	106.90	111.64
2	E	358	MET	N-CA-CB	5.78	120.22	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	33	LEU	N-CA-CB	5.77	120.24	110.49
3	G	130	GLU	CB-CG-CD	5.77	122.41	112.60
2	D	313	PRO	N-CA-CB	5.77	108.46	103.27
2	D	404	VAL	N-CA-C	5.76	115.89	110.30
1	C	246	ALA	O-C-N	-5.73	115.11	120.55
1	B	98	PRO	CA-C-O	-5.72	114.69	121.67
1	C	119	GLY	CA-C-N	5.72	125.74	119.90
1	C	119	GLY	C-N-CA	5.72	125.74	119.90
1	A	119	GLY	CA-C-N	5.71	125.64	119.76
1	A	119	GLY	C-N-CA	5.71	125.64	119.76
1	A	57	SER	CA-C-N	-5.71	116.65	123.44
1	A	57	SER	C-N-CA	-5.71	116.65	123.44
2	F	87	GLY	CA-C-N	5.71	125.38	119.56
2	F	87	GLY	C-N-CA	5.71	125.38	119.56
2	F	461	GLY	CA-C-N	5.69	125.67	120.21
2	F	461	GLY	C-N-CA	5.69	125.67	120.21
1	A	485	THR	N-CA-C	5.68	118.68	111.69
2	F	261	PHE	CA-C-O	5.61	126.71	120.82
1	A	466	ASN	CA-CB-CG	5.59	118.19	112.60
2	D	275	ILE	N-CA-C	-5.59	103.82	108.63
2	D	207	ASN	CA-CB-CG	-5.59	107.01	112.60
1	B	65	ASN	CA-C-O	-5.58	114.39	120.36
1	B	340	THR	N-CA-CB	5.55	118.38	110.16
3	G	39	LYS	CA-C-N	5.54	124.89	118.85
3	G	39	LYS	C-N-CA	5.54	124.89	118.85
1	B	337	TYR	N-CA-C	5.53	116.98	111.07
2	D	221	GLN	OE1-CD-NE2	-5.53	117.08	122.60
2	E	84	ILE	CA-C-N	5.51	125.78	119.83
2	E	84	ILE	C-N-CA	5.51	125.78	119.83
2	E	106	GLY	CA-C-N	5.50	125.50	119.89
2	E	106	GLY	C-N-CA	5.50	125.50	119.89
3	G	75	ARG	CA-C-O	5.48	128.75	121.46
2	F	261	PHE	CA-CB-CG	5.48	119.28	113.80
1	A	203	TYR	CA-C-N	-5.45	115.92	122.90
1	A	203	TYR	C-N-CA	-5.45	115.92	122.90
1	A	75	VAL	N-CA-C	5.43	116.06	108.89
1	C	287	ARG	CA-C-N	5.42	125.97	120.38
1	C	287	ARG	C-N-CA	5.42	125.97	120.38
4	H	87	ASP	N-CA-C	-5.40	102.28	110.28
2	F	96	ASN	CA-CB-CG	5.40	118.00	112.60
2	F	441	PHE	CA-CB-CG	-5.40	108.40	113.80
1	C	338	ILE	CA-C-O	5.38	122.30	118.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	486	ASP	N-CA-C	-5.38	106.22	112.89
1	C	168	ILE	N-CA-C	5.38	116.41	108.45
2	F	357	ILE	CA-CB-CG2	5.38	119.64	110.50
2	D	107	PRO	N-CA-CB	5.37	108.02	103.35
5	I	12	ILE	CA-C-O	5.36	126.53	120.95
2	F	31	PRO	N-CA-CB	5.36	108.43	103.39
1	B	503	ASN	CA-CB-CG	-5.35	107.25	112.60
1	A	172	GLN	CB-CG-CD	5.34	121.68	112.60
2	D	38	VAL	N-CA-CB	5.34	116.35	110.53
1	A	318	GLY	CA-C-N	5.33	127.99	121.06
1	A	318	GLY	C-N-CA	5.33	127.99	121.06
2	F	30	PRO	CA-C-N	5.33	125.62	119.92
2	F	30	PRO	C-N-CA	5.33	125.62	119.92
2	F	144	ALA	CA-C-N	5.33	125.25	119.76
2	F	144	ALA	C-N-CA	5.33	125.25	119.76
1	B	291	ARG	CG-CD-NE	-5.31	100.31	112.00
2	F	80	ALA	N-CA-CB	-5.31	105.82	111.29
1	B	414	THR	N-CA-C	-5.31	105.61	111.71
2	D	87	GLY	CA-C-N	5.31	125.12	119.28
2	D	87	GLY	C-N-CA	5.31	125.12	119.28
3	G	105	ILE	N-CA-C	5.30	116.49	108.96
5	I	5	ARG	N-CA-C	-5.29	103.90	110.41
2	F	274	ARG	NE-CZ-NH1	-5.29	116.21	121.50
2	D	172	ASN	N-CA-C	5.28	118.19	111.69
1	B	119	GLY	CA-C-N	5.28	125.28	119.89
1	B	119	GLY	C-N-CA	5.28	125.28	119.89
2	D	474	ALA	CA-C-N	5.28	131.20	121.70
2	D	474	ALA	C-N-CA	5.28	131.20	121.70
2	F	365	SER	N-CA-C	5.28	117.78	111.71
2	F	249	GLN	N-CA-C	5.27	118.66	110.17
2	E	289	MET	CA-C-N	5.27	125.79	119.94
2	E	289	MET	C-N-CA	5.27	125.79	119.94
2	D	97	VAL	CA-C-N	-5.27	115.73	122.26
2	D	97	VAL	C-N-CA	-5.27	115.73	122.26
3	G	101	LYS	CA-C-N	5.26	131.59	121.54
3	G	101	LYS	C-N-CA	5.26	131.59	121.54
2	D	328	HIS	CA-CB-CG	-5.25	108.55	113.80
1	A	285	LEU	N-CA-C	-5.25	106.66	113.16
1	B	29	GLY	CA-C-O	-5.23	116.46	121.38
1	B	158	PRO	N-CA-CB	5.22	107.96	103.31
1	B	367	VAL	CB-CA-C	-5.22	105.29	111.97
2	E	143	LEU	N-CA-C	5.22	119.73	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	SER	CA-C-O	-5.21	115.35	120.98
1	B	91	THR	N-CA-CB	5.21	117.91	110.67
1	A	210	ARG	CA-C-O	-5.20	115.04	120.55
1	C	457	GLU	CA-C-N	5.18	125.22	119.32
1	C	457	GLU	C-N-CA	5.18	125.22	119.32
2	F	372	ARG	CD-NE-CZ	5.18	131.65	124.40
2	D	51	GLN	OE1-CD-NE2	-5.17	117.43	122.60
4	H	58	LEU	N-CA-C	5.17	116.77	110.41
2	D	106	GLY	CA-C-N	5.15	125.09	119.78
2	D	106	GLY	C-N-CA	5.15	125.09	119.78
2	D	359	ASP	CA-CB-CG	5.15	117.75	112.60
3	G	46	VAL	N-CA-C	-5.15	105.47	110.42
1	C	185	ASN	CA-CB-CG	-5.15	107.45	112.60
2	E	248	GLY	N-CA-C	5.14	120.99	113.48
3	G	137	THR	N-CA-C	5.14	116.80	109.14
2	F	210	ASP	CB-CA-C	-5.14	101.33	111.60
2	F	225	PRO	N-CA-CB	5.13	108.06	103.08
1	C	236	ALA	N-CA-C	5.13	117.61	111.71
2	F	433	PRO	N-CA-CB	5.11	107.80	103.35
4	H	87	ASP	CA-C-O	-5.11	115.44	121.16
2	E	461	GLY	CA-C-N	5.10	125.00	119.85
2	E	461	GLY	C-N-CA	5.10	125.00	119.85
2	D	453	PRO	N-CA-CB	5.09	107.78	103.35
1	B	291	ARG	CA-C-O	-5.08	115.42	120.96
2	D	260	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	A	439	GLU	CB-CG-CD	5.07	121.22	112.60
3	G	78	CYS	N-CA-C	-5.06	105.15	113.50
3	G	116	LEU	N-CA-C	5.05	118.87	111.34
1	A	403	PHE	CA-CB-CG	5.05	118.85	113.80
2	D	64	ASP	CA-C-O	-5.05	115.91	121.31
1	C	367	VAL	CB-CA-C	-5.05	105.51	111.97
1	C	93	ALA	N-CA-C	5.04	117.12	108.90
2	E	251	VAL	CB-CA-C	-5.04	104.32	111.38
2	D	312	VAL	CB-CA-C	-5.04	106.29	111.08
2	F	54	GLY	N-CA-C	-5.04	106.23	112.33
1	C	333	ASP	CA-CB-CG	-5.03	107.57	112.60
2	D	275	ILE	CB-CA-C	-5.03	106.26	110.94
2	E	87	GLY	CA-C-N	5.03	124.81	119.28
2	E	87	GLY	C-N-CA	5.03	124.81	119.28
5	I	39	GLY	N-CA-C	-5.03	104.87	112.41
1	C	137	ILE	CB-CA-C	-5.02	107.42	114.00
1	A	241	PRO	N-CA-CB	5.01	108.81	103.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	244	ARG	CA-C-N	5.01	128.67	121.71
2	F	244	ARG	C-N-CA	5.01	128.67	121.71
2	D	282	GLN	CA-C-N	5.01	124.50	119.19
2	D	282	GLN	C-N-CA	5.01	124.50	119.19

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	3705	0	3809	42	0
1	B	3656	0	3765	70	0
1	C	3718	0	3818	60	0
2	D	3539	0	3592	56	0
2	E	3447	0	3495	118	0
2	F	3530	0	3586	64	0
3	G	1891	0	1971	131	0
4	H	662	0	654	40	0
5	I	281	0	297	26	0
6	A	27	0	12	0	0
6	B	27	0	12	0	0
6	C	27	0	12	0	0
6	D	27	0	12	0	0
6	E	27	0	12	0	0
6	F	27	0	12	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	A	6	0	8	0	0
8	B	12	0	15	1	0
8	C	6	0	8	1	0
9	D	5	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	5	0	0	0	0
10	E	5	0	0	0	0
11	A	310	0	0	2	0
11	B	241	0	0	5	0
11	C	322	0	0	6	0
11	D	310	0	0	4	0
11	E	181	0	0	3	0
11	F	286	0	0	4	0
11	G	39	0	0	2	0
11	H	3	0	0	0	0
11	I	1	0	0	0	0
All	All	26329	0	25090	572	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 12.

All (572) 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:F:130:GLN:HB3	2:F:357:ILE:HD11	1.27	1.12
3:G:130:GLU:HG3	5:I:41:THR:HG22	1.30	1.08
3:G:75:ARG:HG2	3:G:76:GLY:H	1.25	1.01
2:D:382:LYS:HA	2:D:385:GLN:HE21	1.27	0.98
3:G:28:ALA:HA	3:G:229:MET:HE2	1.47	0.97
2:D:282:GLN:H	2:D:282:GLN:HE21	1.01	0.95
2:F:136:GLY:HA3	2:F:431:LEU:HD12	1.47	0.94
2:F:282:GLN:H	2:F:282:GLN:HE21	0.99	0.93
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.52	0.92
1:C:381:ARG:HH11	1:C:488:LYS:HZ3	1.19	0.90
2:E:282:GLN:H	2:E:282:GLN:HE21	1.21	0.89
2:E:97:VAL:HB	2:E:232:VAL:HG12	1.55	0.87
2:E:133:LEU:HD11	2:E:252:LEU:HD21	1.56	0.86
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.58	0.86
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.07	0.83
1:C:381:ARG:HH11	1:C:488:LYS:NZ	1.76	0.83
2:D:387:ILE:HG13	3:G:16:ILE:HD13	1.59	0.82
2:E:455:GLN:C	2:E:457:PHE:H	1.87	0.82
3:G:85:VAL:HG12	3:G:89:MET:HE2	1.59	0.81
2:F:10:THR:HG22	2:F:76:LEU:HD22	1.61	0.81
3:G:20:THR:HA	3:G:23:MET:HE3	1.65	0.79
2:E:138:LYS:HD2	2:E:432:VAL:HG21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:MET:HE1	2:D:196:LEU:HD13	1.65	0.78
2:F:131:GLU:HG2	2:F:148:LYS:HD2	1.66	0.78
3:G:197:ASP:H	3:G:200:VAL:HG12	1.47	0.78
1:C:390:MET:HE3	1:C:424:LEU:HD13	1.65	0.78
2:F:394:ASP:HB3	3:G:79:GLY:HA3	1.66	0.76
2:E:169:LEU:O	2:E:173:VAL:HG22	1.83	0.76
3:G:76:GLY:HA3	3:G:228:ARG:NH2	2.00	0.76
1:B:65:ASN:ND2	2:F:17:ILE:HD13	1.99	0.76
2:F:388:ILE:HD11	2:F:396:LEU:HD22	1.67	0.76
2:F:282:GLN:HE21	2:F:282:GLN:N	1.82	0.76
2:D:136:GLY:HA3	2:D:431:LEU:HD13	1.69	0.75
3:G:76:GLY:HA3	3:G:228:ARG:HH21	1.49	0.75
3:G:197:ASP:H	3:G:200:VAL:CG1	2.00	0.75
2:E:148:LYS:HE2	2:E:250:ASP:HB3	1.68	0.75
3:G:129:LYS:HE2	5:I:43:LYS:HG2	1.67	0.75
3:G:192:ILE:HG22	4:H:53:PRO:HG2	1.68	0.75
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.51	0.75
2:F:245:ASP:C	2:F:247:GLU:H	1.96	0.74
2:F:196:LEU:HD11	2:F:200:MET:HE3	1.69	0.74
1:C:185:ASN:OD1	1:C:188:ARG:NH1	2.21	0.74
3:G:179:PHE:O	3:G:181:LEU:N	2.21	0.73
1:A:423:ARG:HG2	1:A:461:ILE:HD11	1.71	0.73
3:G:87:LYS:HA	3:G:90:LYS:HE2	1.68	0.73
1:B:508:PHE:CZ	1:B:510:ALA:HB3	2.24	0.72
5:I:5:ARG:C	5:I:7:ALA:H	1.95	0.72
1:A:376:SER:HB3	1:A:384:LYS:HD3	1.70	0.72
1:B:78:ASN:HD21	1:B:80:LYS:HE2	1.53	0.72
2:D:223:ASN:H	2:D:223:ASN:HD22	1.37	0.72
1:C:52:MET:HE2	1:C:60:LYS:HB3	1.70	0.71
2:E:220:GLY:HA3	2:E:232:VAL:HG11	1.72	0.71
3:G:89:MET:HE1	3:G:112:ILE:HG23	1.72	0.71
3:G:167:SER:OG	3:G:170:SER:HB3	1.91	0.71
1:A:286:ARG:NH2	3:G:272:LEU:HD13	2.05	0.70
1:B:460:LYS:HZ2	1:B:510:ALA:HB1	1.56	0.70
3:G:75:ARG:CG	3:G:76:GLY:H	1.98	0.70
3:G:51:LEU:HD13	4:H:55:LEU:HD21	1.73	0.70
3:G:166:ARG:NH2	3:G:172:LYS:HD3	2.06	0.70
1:B:479:LEU:HA	1:B:482:LYS:HD2	1.72	0.70
2:D:473:LEU:C	2:D:475:GLU:H	1.99	0.70
1:C:354:THR:HG23	11:C:2111:HOH:O	1.91	0.69
2:E:174:ALA:HB2	11:E:2078:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:82:HIS:CD2	3:G:111:LYS:HG2	2.27	0.69
2:D:382:LYS:HA	2:D:385:GLN:NE2	2.05	0.69
1:B:37:GLY:O	11:B:2005:HOH:O	2.10	0.69
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.73	0.68
2:D:282:GLN:H	2:D:282:GLN:NE2	1.84	0.68
4:H:48:LEU:C	4:H:50:ALA:H	2.02	0.68
4:H:48:LEU:HD13	4:H:49:ALA:N	2.08	0.68
4:H:48:LEU:O	4:H:50:ALA:N	2.27	0.68
1:A:180:ILE:CD1	1:A:216:LEU:HD21	2.23	0.68
3:G:19:ILE:HG22	3:G:23:MET:HE2	1.75	0.68
4:H:34:ARG:HE	4:H:66:HIS:HB3	1.59	0.68
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.59	0.68
2:E:455:GLN:C	2:E:457:PHE:N	2.51	0.67
2:F:188:GLU:H	2:F:221:GLN:NE2	1.92	0.67
1:A:487:GLY:O	1:A:488:LYS:HB2	1.93	0.67
1:B:381:ARG:O	1:B:385:GLN:HG3	1.95	0.67
3:G:77:LEU:HD12	3:G:232:MET:HE1	1.75	0.67
4:H:22:SER:HB2	4:H:23:PRO:HD2	1.76	0.67
1:C:52:MET:HE1	1:C:76:PHE:CD1	2.30	0.67
1:C:171:ARG:HD2	11:C:2114:HOH:O	1.95	0.66
2:E:228:ALA:O	2:E:232:VAL:HG13	1.95	0.66
2:E:172:ASN:ND2	2:E:431:LEU:HD13	2.10	0.66
2:E:410:ILE:HG13	2:E:444:ILE:HG21	1.78	0.66
3:G:106:ILE:HD11	3:G:148:LEU:HD13	1.76	0.66
4:H:58:LEU:HD11	4:H:92:LEU:HD11	1.78	0.66
3:G:127:THR:OG1	5:I:45:VAL:HB	1.95	0.65
3:G:71:VAL:HA	3:G:108:VAL:HG22	1.78	0.65
2:E:388:ILE:HG23	2:E:393:MET:HB2	1.78	0.65
2:E:200:MET:SD	2:E:205:VAL:HG21	2.37	0.65
4:H:65:VAL:C	4:H:72:THR:HG23	2.22	0.65
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.78	0.64
2:E:131:GLU:HG2	2:E:132:ILE:H	1.61	0.64
3:G:87:LYS:O	3:G:90:LYS:HG2	1.96	0.64
3:G:207:TYR:HA	5:I:12:ILE:HD11	1.79	0.64
1:C:362:ARG:HA	1:C:363:PRO:C	2.22	0.64
3:G:39:LYS:N	3:G:40:PRO:HD2	2.13	0.64
2:E:348:VAL:O	2:E:350:PRO:HD3	1.97	0.64
4:H:85:ASN:HD21	4:H:91:GLN:HE22	1.43	0.64
3:G:75:ARG:HG2	3:G:76:GLY:N	2.06	0.63
1:C:218:LYS:HD2	2:F:128:VAL:HG21	1.81	0.63
2:E:447:GLY:C	2:E:449:TYR:H	2.03	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LEU:O	1:B:422:VAL:HG23	1.99	0.63
2:D:245:ASP:C	2:D:247:GLU:H	2.07	0.63
2:E:310:ILE:HD13	2:E:325:THR:HG21	1.80	0.63
3:G:130:GLU:HG3	5:I:41:THR:CG2	2.20	0.63
1:A:185:ASN:OD1	1:A:435:PRO:HB2	1.99	0.63
1:B:412:ALA:HA	1:B:415:GLN:HB3	1.80	0.63
2:E:220:GLY:CA	2:E:232:VAL:HG11	2.29	0.62
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.34	0.62
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.80	0.62
2:E:443:GLN:O	2:E:444:ILE:C	2.42	0.62
1:B:509:GLU:O	1:B:510:ALA:C	2.43	0.62
2:E:452:LEU:HD11	2:E:456:ALA:HB3	1.82	0.62
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.35	0.62
2:F:223:ASN:HD22	2:F:223:ASN:H	1.47	0.62
3:G:19:ILE:CG2	3:G:23:MET:HE2	2.30	0.62
3:G:82:HIS:CG	3:G:111:LYS:HG2	2.34	0.62
3:G:85:VAL:HG13	3:G:161:ILE:HG22	1.81	0.62
4:H:65:VAL:O	4:H:72:THR:HG23	2.00	0.62
1:C:452:TYR:OH	1:C:498:LYS:HG3	2.00	0.62
1:B:65:ASN:HD22	2:F:17:ILE:HD13	1.62	0.61
3:G:49:LEU:HD21	3:G:212:ILE:HD12	1.80	0.61
2:D:25:PHE:HB2	2:D:29:LEU:HD23	1.81	0.61
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.81	0.61
2:E:370:VAL:HG21	2:E:438:ILE:HG23	1.81	0.61
1:B:497:LEU:O	1:B:501:VAL:HG23	2.01	0.61
1:B:478:ALA:O	1:B:482:LYS:HG3	2.01	0.61
2:F:171:ASN:HA	2:F:175:LYS:HD2	1.82	0.61
2:E:112:GLN:C	2:E:113:PHE:CD2	2.79	0.60
2:D:458:TYR:CE2	2:D:459:MET:HG2	2.37	0.60
2:D:244:ARG:O	2:D:248:GLY:HA2	2.00	0.60
3:G:180:SER:O	3:G:181:LEU:C	2.44	0.60
1:A:187:LYS:NZ	1:A:224:ASP:HB3	2.17	0.60
4:H:85:ASN:HD21	4:H:91:GLN:NE2	1.98	0.60
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.84	0.60
2:E:143:LEU:HD12	2:E:350:PRO:HB3	1.84	0.59
1:A:360:GLY:HA2	1:A:362:ARG:NH1	2.17	0.59
1:C:23:VAL:HG12	1:C:23:VAL:O	2.02	0.59
2:E:444:ILE:O	2:E:445:LEU:C	2.45	0.59
2:F:282:GLN:H	2:F:282:GLN:NE2	1.84	0.59
3:G:111:LYS:O	3:G:115:ILE:HG13	2.03	0.59
2:E:148:LYS:CE	2:E:250:ASP:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:70:GLY:O	4:H:71:THR:C	2.45	0.59
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.85	0.59
2:E:355:SER:C	2:E:357:ILE:H	2.10	0.59
2:E:429:GLY:C	2:E:430:LYS:HG2	2.28	0.59
2:E:170:ILE:CG2	2:E:215:VAL:HG21	2.34	0.58
3:G:21:LYS:HG2	3:G:236:SER:HB2	1.85	0.58
2:D:387:ILE:HG13	3:G:16:ILE:CD1	2.30	0.58
2:E:330:ASP:HA	2:E:356:ARG:HD2	1.83	0.58
1:C:45:ARG:NH2	1:C:68:PRO:O	2.35	0.58
3:G:82:HIS:HB3	3:G:115:ILE:CD1	2.33	0.58
3:G:105:ILE:HG22	3:G:106:ILE:N	2.18	0.58
4:H:47:ILE:HG21	4:H:90:VAL:HG21	1.85	0.58
1:B:416:GLN:HG2	1:B:417:LEU:N	2.18	0.58
4:H:78:SER:HB2	5:I:18:CYS:C	2.29	0.58
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.85	0.58
3:G:128:PHE:HE2	5:I:44:ILE:HD13	1.69	0.58
1:B:209:LYS:HZ2	2:E:356:ARG:HH12	1.52	0.58
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.19	0.58
1:B:183:ILE:HD11	1:B:267:ILE:HD12	1.86	0.58
1:B:187:LYS:HE3	1:B:224:ASP:HB3	1.85	0.58
1:B:463:LYS:NZ	1:B:510:ALA:HB2	2.18	0.58
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.85	0.58
2:F:252:LEU:HD23	2:F:305:THR:HB	1.86	0.58
3:G:39:LYS:HB2	3:G:40:PRO:CD	2.34	0.57
4:H:48:LEU:C	4:H:50:ALA:N	2.61	0.57
5:I:5:ARG:O	5:I:6:GLN:HB3	2.04	0.57
3:G:179:PHE:C	3:G:181:LEU:N	2.61	0.57
4:H:36:VAL:O	4:H:46:GLY:HA2	2.04	0.57
1:A:19:ALA:O	1:A:22:SER:HB3	2.04	0.57
1:A:23:VAL:HG21	1:A:30:ARG:NH2	2.20	0.57
2:E:388:ILE:HG23	2:E:393:MET:CB	2.34	0.57
3:G:164:ARG:HA	3:G:219:GLU:HG2	1.87	0.57
2:F:266:SER:HB3	2:F:282:GLN:HE22	1.69	0.56
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.34	0.56
2:E:173:VAL:HG23	11:E:2076:HOH:O	2.04	0.56
1:B:362:ARG:HA	1:B:363:PRO:C	2.30	0.56
1:B:436:MET:HE3	1:B:469:LEU:HD21	1.86	0.56
2:E:366:GLU:HG3	2:E:367:HIS:H	1.71	0.56
1:C:194:ASP:OD2	1:C:197:LYS:HG3	2.06	0.56
3:G:23:MET:CE	3:G:232:MET:HE3	2.35	0.56
1:C:263:HIS:HD2	1:C:320:SER:OG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:174:ALA:O	2:F:177:HIS:HB3	2.07	0.55
3:G:116:LEU:O	3:G:117:HIS:C	2.49	0.55
4:H:40:THR:HG23	4:H:56:GLN:HB3	1.88	0.55
1:B:209:LYS:NZ	2:E:356:ARG:HH12	2.04	0.55
2:D:196:LEU:HD11	2:D:200:MET:HE3	1.88	0.55
1:A:362:ARG:HA	1:A:363:PRO:C	2.30	0.55
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.42	0.55
3:G:207:TYR:HA	5:I:12:ILE:CD1	2.37	0.55
1:B:479:LEU:HD23	1:B:496:LYS:HD3	1.88	0.55
3:G:164:ARG:NH1	3:G:174:GLU:OE2	2.40	0.55
3:G:164:ARG:HD3	3:G:174:GLU:OE2	2.07	0.55
1:B:34:ILE:HD11	1:B:79:ASP:CB	2.35	0.54
1:B:390:MET:HE1	1:B:445:ILE:HD12	1.89	0.54
2:D:458:TYR:CZ	2:D:459:MET:HG2	2.43	0.54
1:C:390:MET:HE3	1:C:424:LEU:HD22	1.88	0.54
2:E:200:MET:HB3	2:E:206:ILE:HG13	1.89	0.54
3:G:74:ASP:OD1	3:G:110:ASP:N	2.37	0.54
1:C:179:ALA:HB1	1:C:267:ILE:HG12	1.88	0.54
5:I:5:ARG:C	5:I:7:ALA:N	2.61	0.54
1:B:410:LEU:HG	1:B:411:ASP:H	1.73	0.54
4:H:64:VAL:HG12	4:H:72:THR:CG2	2.36	0.54
3:G:75:ARG:CG	3:G:76:GLY:N	2.65	0.54
2:D:44:ARG:HD3	11:D:2020:HOH:O	2.08	0.54
2:E:447:GLY:C	2:E:449:TYR:N	2.61	0.54
1:C:172:GLN:O	1:C:172:GLN:HG3	2.07	0.54
2:E:370:VAL:HG21	2:E:438:ILE:CG2	2.38	0.53
2:F:398:GLU:HA	2:F:401:LYS:HB2	1.90	0.53
3:G:128:PHE:CE2	5:I:44:ILE:HD13	2.43	0.53
3:G:15:ASN:OD1	3:G:16:ILE:N	2.41	0.53
3:G:23:MET:SD	3:G:232:MET:HE3	2.48	0.53
2:F:245:ASP:C	2:F:247:GLU:N	2.62	0.53
5:I:13:ARG:NH1	5:I:16:GLN:NE2	2.56	0.53
1:C:240:ALA:N	1:C:241:PRO:CD	2.71	0.53
3:G:51:LEU:CD1	4:H:55:LEU:HD21	2.37	0.53
3:G:190:MET:HE2	3:G:193:TYR:CE1	2.43	0.53
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.90	0.53
2:E:408:ARG:NH1	2:E:454:GLU:OE2	2.41	0.53
3:G:139:GLY:O	3:G:143:VAL:HG23	2.08	0.53
1:B:78:ASN:HD21	1:B:80:LYS:CE	2.20	0.53
1:A:52:MET:HG3	1:A:95:VAL:CG2	2.39	0.53
1:C:52:MET:HE1	1:C:76:PHE:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:67:LEU:HD12	3:G:104:LYS:O	2.07	0.53
4:H:59:ARG:HG2	4:H:60:PRO:HD2	1.91	0.53
2:E:404:VAL:O	2:E:408:ARG:HG3	2.10	0.52
2:E:452:LEU:HD12	2:E:457:PHE:CE1	2.43	0.52
1:B:105:GLY:HA2	1:B:226:MET:O	2.09	0.52
2:E:355:SER:C	2:E:357:ILE:N	2.65	0.52
3:G:179:PHE:O	3:G:180:SER:C	2.52	0.52
2:F:25:PHE:HB2	2:F:29:LEU:HD23	1.90	0.52
1:A:218:LYS:HG3	2:D:128:VAL:HG21	1.91	0.52
2:E:374:VAL:HG13	2:E:410:ILE:HG21	1.92	0.52
2:E:337:ARG:O	2:E:341:GLU:HG2	2.10	0.52
2:F:167:MET:HE3	11:F:2067:HOH:O	2.09	0.52
3:G:76:GLY:HA3	3:G:228:ARG:CZ	2.39	0.52
2:E:394:ASP:C	2:E:396:LEU:H	2.18	0.52
2:F:393:MET:SD	2:F:404:VAL:HG11	2.49	0.52
3:G:82:HIS:HB3	3:G:115:ILE:HD11	1.92	0.52
1:A:487:GLY:O	1:A:488:LYS:CB	2.58	0.51
1:B:97:VAL:HB	1:B:98:PRO:HD2	1.92	0.51
1:B:209:LYS:NZ	2:E:356:ARG:NH1	2.58	0.51
1:B:351:PHE:HE1	1:B:369:LEU:O	1.92	0.51
2:E:187:GLY:O	2:E:222:MET:HE2	2.10	0.51
2:E:412:ARG:HB3	2:E:458:TYR:HA	1.92	0.51
2:F:388:ILE:O	2:F:389:ALA:C	2.53	0.51
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.43	0.51
1:C:381:ARG:HD3	1:C:488:LYS:NZ	2.25	0.51
2:E:252:LEU:HD22	2:E:305:THR:HB	1.90	0.51
2:E:364:GLY:O	2:E:365:SER:C	2.52	0.51
4:H:51:HIS:ND1	4:H:52:VAL:O	2.36	0.51
1:B:479:LEU:HA	1:B:482:LYS:CD	2.41	0.51
1:B:45:ARG:NH2	1:B:68:PRO:O	2.33	0.51
2:D:89:GLU:HG2	2:D:109:LYS:O	2.10	0.51
2:E:25:PHE:HB2	2:E:29:LEU:HD23	1.93	0.51
2:F:357:ILE:HD13	2:F:362:ILE:HD13	1.93	0.51
1:A:136:ILE:HD13	2:E:190:THR:HG23	1.93	0.51
1:B:463:LYS:HD3	1:B:510:ALA:CB	2.41	0.51
1:C:129:VAL:HG23	8:C:602:GOL:H12	1.93	0.51
2:E:360:PRO:HD3	2:E:368:TYR:CE1	2.46	0.51
3:G:131:VAL:C	3:G:133:ARG:H	2.20	0.51
3:G:167:SER:HG	3:G:170:SER:HB3	1.76	0.50
2:F:357:ILE:CD1	2:F:362:ILE:HG21	2.40	0.50
5:I:20:LYS:O	5:I:23:ARG:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:416:GLN:HG3	2:E:417:PRO:HD2	1.93	0.50
2:F:223:ASN:HD22	2:F:223:ASN:N	2.07	0.50
2:D:249:GLN:O	2:D:251:VAL:HG23	2.11	0.50
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.94	0.50
2:E:447:GLY:O	2:E:449:TYR:N	2.45	0.50
2:F:245:ASP:O	2:F:247:GLU:N	2.45	0.50
3:G:15:ASN:OD1	3:G:15:ASN:C	2.55	0.50
3:G:17:GLN:OE1	3:G:240:SER:N	2.44	0.50
1:B:410:LEU:HG	1:B:411:ASP:N	2.27	0.50
2:F:454:GLU:HG3	11:F:2277:HOH:O	2.12	0.50
3:G:26:VAL:O	3:G:29:ALA:N	2.44	0.50
4:H:64:VAL:HG12	4:H:72:THR:HG21	1.92	0.50
1:C:356:LEU:HB3	1:C:361:ILE:HB	1.94	0.50
1:A:25:LEU:HD23	1:A:25:LEU:N	2.27	0.49
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.93	0.49
1:C:168:ILE:HD11	1:C:339:PRO:HB3	1.94	0.49
3:G:52:TYR:CD2	3:G:57:ILE:HD12	2.46	0.49
2:E:345:TYR:HA	2:E:346:PRO:C	2.36	0.49
1:A:157:VAL:N	1:A:158:PRO:CD	2.74	0.49
3:G:115:ILE:HG22	3:G:115:ILE:O	2.13	0.49
4:H:35:GLN:HB3	4:H:66:HIS:CD2	2.47	0.49
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.47	0.49
2:E:410:ILE:CG1	2:E:444:ILE:HG21	2.42	0.49
3:G:105:ILE:CG2	3:G:106:ILE:N	2.75	0.49
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	0.49
3:G:244:ASP:O	3:G:248:LEU:HG	2.11	0.49
1:A:186:GLN:HG3	1:A:199:LEU:HD23	1.95	0.49
1:C:171:ARG:NH1	11:C:2112:HOH:O	2.45	0.49
2:E:223:ASN:HD22	2:E:223:ASN:H	1.60	0.49
4:H:99:THR:O	4:H:102:MET:HG2	2.13	0.49
1:C:52:MET:HE3	1:C:61:GLY:O	2.13	0.49
1:A:414:THR:HG21	2:E:389:ALA:HB1	1.94	0.49
1:B:54:GLU:HG2	1:B:60:LYS:CD	2.43	0.49
2:F:455:GLN:O	2:F:469:LYS:HE2	2.13	0.49
1:A:291:ARG:HG2	1:A:292:GLU:HG3	1.95	0.48
2:D:196:LEU:O	2:D:200:MET:HG3	2.13	0.48
3:G:133:ARG:HG2	11:G:2013:HOH:O	2.13	0.48
4:H:85:ASN:ND2	4:H:91:GLN:HE22	2.11	0.48
3:G:184:ILE:HD13	3:G:184:ILE:O	2.14	0.48
5:I:13:ARG:HH11	5:I:16:GLN:NE2	2.10	0.48
2:F:419:GLN:O	2:F:422:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:37:GLU:OE2	3:G:218:LYS:NZ	2.46	0.48
5:I:37:THR:HG22	5:I:38:SER:H	1.78	0.48
1:B:463:LYS:HD3	1:B:510:ALA:HB2	1.95	0.48
2:F:345:TYR:HA	2:F:346:PRO:C	2.39	0.48
2:E:455:GLN:O	2:E:457:PHE:N	2.46	0.48
3:G:181:LEU:HD23	3:G:184:ILE:H	1.79	0.48
4:H:35:GLN:HB3	4:H:66:HIS:HD2	1.78	0.48
2:E:449:TYR:HB3	2:E:452:LEU:HB3	1.95	0.48
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.95	0.48
2:D:158:ALA:HA	9:D:620:ALF:F1	2.03	0.48
2:E:276:PRO:HD2	3:G:266:ILE:HD11	1.96	0.48
2:E:439:LYS:HE2	2:E:443:GLN:NE2	2.28	0.48
3:G:81:ILE:HG22	3:G:82:HIS:N	2.28	0.48
5:I:5:ARG:O	5:I:6:GLN:CB	2.59	0.48
1:C:52:MET:HE1	1:C:76:PHE:HD1	1.75	0.48
2:E:359:ASP:OD1	2:E:360:PRO:HD2	2.14	0.47
3:G:162:PHE:O	3:G:173:THR:HA	2.14	0.47
3:G:181:LEU:HD23	3:G:184:ILE:N	2.29	0.47
2:E:97:VAL:HB	2:E:232:VAL:CG1	2.37	0.47
3:G:185:SER:CB	3:G:205:GLN:HE21	2.27	0.47
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.96	0.47
3:G:129:LYS:O	3:G:130:GLU:CB	2.62	0.47
3:G:203:ASN:OD1	5:I:5:ARG:NH2	2.43	0.47
1:C:224:ASP:O	1:C:227:LYS:HE2	2.14	0.47
2:E:388:ILE:HG12	2:E:396:LEU:HD11	1.97	0.47
4:H:40:THR:CG2	4:H:56:GLN:HB3	2.45	0.47
1:C:97:VAL:HB	1:C:98:PRO:HD2	1.97	0.47
2:E:126:MET:HE3	2:E:126:MET:HB2	1.79	0.47
1:B:185:ASN:O	1:B:188:ARG:HD2	2.14	0.47
2:E:95:MET:HG3	2:E:99:GLY:HA2	1.95	0.47
2:F:408:ARG:HE	2:F:454:GLU:CD	2.22	0.47
1:C:26:GLU:HB3	1:C:46:ASN:ND2	2.30	0.47
3:G:26:VAL:O	3:G:27:ALA:C	2.57	0.47
3:G:36:ARG:O	3:G:39:LYS:HG3	2.14	0.47
3:G:189:SER:O	3:G:192:ILE:HD12	2.14	0.47
2:D:50:ALA:C	2:D:51:GLN:HG3	2.39	0.47
9:D:620:ALF:F4	11:D:2121:HOH:O	2.10	0.47
5:I:4:TRP:HB2	5:I:9:LEU:HB2	1.96	0.47
1:A:216:LEU:O	1:A:216:LEU:HD22	2.14	0.47
1:B:453:LEU:O	1:B:456:LEU:HB2	2.15	0.47
2:D:360:PRO:HD3	2:D:368:TYR:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:33:ARG:O	3:G:34:ALA:C	2.58	0.47
1:A:338:ILE:N	1:A:339:PRO:CD	2.78	0.46
1:C:137:ILE:HB	1:C:138:PRO:HD3	1.97	0.46
2:D:245:ASP:C	2:D:247:GLU:N	2.71	0.46
2:E:63:MET:HE1	2:E:231:ARG:HB2	1.96	0.46
4:H:40:THR:HG22	4:H:41:GLN:N	2.30	0.46
4:H:98:VAL:HG21	4:H:103:LEU:HD21	1.96	0.46
1:A:240:ALA:N	1:A:241:PRO:HD2	2.30	0.46
1:C:429:LYS:NZ	11:C:2264:HOH:O	2.48	0.46
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.98	0.46
2:E:148:LYS:HE3	2:E:305:THR:OG1	2.15	0.46
3:G:107:GLY:HA3	3:G:112:ILE:HG21	1.98	0.46
4:H:87:ASP:O	4:H:89:SER:N	2.48	0.46
2:F:391:LEU:HD13	2:F:395:GLU:HG2	1.98	0.46
1:B:509:GLU:OE1	1:B:509:GLU:HA	2.15	0.46
3:G:75:ARG:O	3:G:82:HIS:HE1	1.98	0.46
1:C:381:ARG:NH1	1:C:488:LYS:NZ	2.56	0.46
3:G:76:GLY:CA	3:G:228:ARG:HH21	2.24	0.46
1:C:80:LYS:HE3	2:F:33:LEU:HD12	1.98	0.46
3:G:33:ARG:O	3:G:36:ARG:N	2.46	0.46
3:G:81:ILE:HG13	3:G:224:GLU:HA	1.96	0.46
1:B:201:CYS:C	1:B:202:ILE:HG13	2.40	0.46
1:B:397:TYR:O	1:B:399:GLU:N	2.49	0.46
2:D:249:GLN:OE1	2:D:249:GLN:HA	2.16	0.46
2:E:422:GLU:HG2	2:E:427:HIS:O	2.16	0.46
2:F:188:GLU:O	2:F:221:GLN:HB3	2.15	0.46
3:G:181:LEU:CD2	3:G:183:THR:HB	2.46	0.46
5:I:44:ILE:HG21	5:I:46:LYS:HE2	1.98	0.46
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.81	0.45
2:E:416:GLN:NE2	2:E:432:VAL:HG23	2.32	0.45
2:D:223:ASN:HD22	2:D:223:ASN:N	2.07	0.45
2:D:348:VAL:O	2:D:350:PRO:HD3	2.16	0.45
3:G:85:VAL:CG1	3:G:89:MET:HE2	2.39	0.45
2:D:52:HIS:CD2	2:D:58:VAL:HG12	2.51	0.45
2:E:266:SER:HB2	2:E:282:GLN:NE2	2.32	0.45
2:E:394:ASP:C	2:E:396:LEU:N	2.75	0.45
2:E:443:GLN:O	2:E:446:ALA:N	2.49	0.45
1:C:469:LEU:HD12	1:C:472:VAL:CG2	2.46	0.45
2:F:249:GLN:OE1	2:F:249:GLN:HA	2.16	0.45
4:H:19:THR:HA	4:H:28:PHE:O	2.17	0.45
1:B:287:ARG:NE	11:B:2149:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:THR:OG1	2:D:76:LEU:HD23	2.16	0.45
3:G:73:SER:HA	3:G:131:VAL:HB	1.98	0.45
3:G:180:SER:O	3:G:182:ASP:N	2.50	0.45
3:G:181:LEU:O	3:G:184:ILE:HG22	2.17	0.45
5:I:4:TRP:H	5:I:4:TRP:CD1	2.34	0.45
1:C:338:ILE:N	1:C:339:PRO:CD	2.79	0.45
3:G:36:ARG:C	3:G:38:LEU:H	2.23	0.45
1:A:23:VAL:HG12	1:A:25:LEU:CD2	2.47	0.45
2:E:314:ALA:O	2:E:315:ASP:HB2	2.15	0.45
3:G:190:MET:HE2	3:G:193:TYR:CD1	2.52	0.45
1:B:101:GLU:OE2	1:B:262:LYS:NZ	2.47	0.45
2:F:348:VAL:O	2:F:350:PRO:HD3	2.17	0.45
2:D:196:LEU:O	2:D:196:LEU:HD12	2.17	0.44
2:D:246:GLN:O	2:D:247:GLU:HG3	2.17	0.44
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.52	0.44
2:F:212:THR:O	2:F:214:LYS:HE2	2.17	0.44
1:A:44:LEU:HB3	1:A:47:VAL:HB	1.99	0.44
1:A:187:LYS:HZ2	1:A:224:ASP:HB3	1.82	0.44
1:C:239:ALA:HB1	1:C:241:PRO:HD2	1.99	0.44
3:G:36:ARG:C	3:G:38:LEU:N	2.75	0.44
1:B:390:MET:CE	1:B:424:LEU:HD22	2.47	0.44
3:G:39:LYS:N	3:G:40:PRO:CD	2.79	0.44
2:E:374:VAL:O	2:E:377:ILE:HG22	2.17	0.44
2:F:223:ASN:H	2:F:223:ASN:ND2	2.15	0.44
3:G:52:TYR:HD2	3:G:57:ILE:HD12	1.81	0.44
2:D:130:GLN:NE2	11:D:2088:HOH:O	2.50	0.44
4:H:38:VAL:HG13	4:H:39:PRO:HD2	1.99	0.44
1:B:140:ILE:HD12	11:B:2077:HOH:O	2.18	0.44
1:C:102:GLU:HG2	1:C:122:GLY:O	2.17	0.44
2:F:166:ILE:HG22	2:F:167:MET:HE2	1.98	0.44
2:E:39:GLN:NE2	2:E:76:LEU:HG	2.32	0.44
3:G:198:ALA:C	3:G:199:ASP:OD1	2.61	0.44
2:D:205:VAL:HG12	2:D:215:VAL:HG23	1.99	0.44
2:E:360:PRO:HG3	2:E:368:TYR:CD2	2.53	0.44
2:F:388:ILE:CD1	2:F:396:LEU:HD22	2.44	0.44
2:E:66:THR:HB	2:E:69:LEU:HD12	2.00	0.44
2:E:418:PHE:O	2:E:419:GLN:C	2.61	0.44
2:E:452:LEU:HA	2:E:453:PRO:HD3	1.87	0.44
3:G:39:LYS:CB	3:G:40:PRO:CD	2.95	0.44
1:A:137:ILE:N	1:A:138:PRO:HD2	2.33	0.43
1:C:83:LYS:NZ	2:F:29:LEU:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ASP:HA	1:C:270:ASP:HA	1.74	0.43
2:F:188:GLU:H	2:F:221:GLN:HE22	1.66	0.43
1:A:410:LEU:HD23	1:A:410:LEU:N	2.33	0.43
2:E:416:GLN:NE2	2:E:430:LYS:O	2.49	0.43
1:B:496:LYS:NZ	11:B:2232:HOH:O	2.50	0.43
8:B:700:GOL:H11	11:F:2286:HOH:O	2.18	0.43
1:C:396:GLN:O	1:C:400:VAL:HG23	2.19	0.43
2:E:359:ASP:OD2	2:E:361:ASN:HB2	2.18	0.43
2:E:452:LEU:CD1	2:E:456:ALA:HB3	2.48	0.43
2:E:384:LEU:O	2:E:387:ILE:HG23	2.19	0.43
3:G:73:SER:OG	3:G:224:GLU:OE2	2.33	0.43
1:A:446:TYR:O	1:A:447:ALA:C	2.60	0.43
2:E:275:ILE:HA	2:E:276:PRO:HD3	1.90	0.43
3:G:72:SER:OG	3:G:82:HIS:HD2	2.01	0.43
1:B:338:ILE:HB	1:B:339:PRO:HD3	2.01	0.43
1:B:446:TYR:O	1:B:447:ALA:C	2.60	0.43
11:B:2153:HOH:O	3:G:263:ILE:HG21	2.18	0.43
2:D:84:ILE:HG21	2:D:235:THR:HG23	2.00	0.43
3:G:164:ARG:NH2	3:G:166:ARG:NE	2.67	0.43
4:H:16:MET:HB3	4:H:49:ALA:HA	1.99	0.43
1:B:35:GLY:O	1:B:36:ASP:HB2	2.19	0.43
2:E:366:GLU:O	2:E:370:VAL:HG23	2.18	0.43
3:G:193:TYR:HB3	3:G:196:ILE:HD11	1.99	0.43
4:H:26:VAL:HG13	4:H:26:VAL:O	2.19	0.43
2:F:471:ASP:O	2:F:474:ALA:N	2.52	0.43
1:A:218:LYS:HE2	1:A:222:ASP:OD2	2.18	0.43
1:C:188:ARG:HH11	1:C:188:ARG:HG2	1.84	0.43
2:D:422:GLU:HG2	2:D:427:HIS:O	2.18	0.43
2:E:122:GLU:H	2:E:125:GLU:CD	2.27	0.43
2:E:445:LEU:O	2:E:446:ALA:C	2.61	0.43
2:F:174:ALA:O	2:F:177:HIS:N	2.51	0.43
1:B:463:LYS:CE	1:B:510:ALA:HB2	2.48	0.42
1:C:137:ILE:HG12	11:D:2065:HOH:O	2.19	0.42
11:C:2191:HOH:O	2:D:226:PRO:HG3	2.18	0.42
2:F:408:ARG:NE	2:F:454:GLU:OE2	2.42	0.42
2:D:37:GLU:CD	2:D:44:ARG:HE	2.28	0.42
2:E:120:ALA:HB1	2:E:121:PRO:HD2	2.00	0.42
2:E:256:ASP:HA	2:E:257:ASN:HA	1.85	0.42
2:E:433:PRO:O	2:E:434:LEU:C	2.63	0.42
3:G:178:ILE:CD1	3:G:212:ILE:HG21	2.50	0.42
2:E:172:ASN:CG	2:E:431:LEU:HD13	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:415:SER:O	2:F:416:GLN:HB2	2.19	0.42
5:I:4:TRP:CZ3	5:I:10:SER:C	2.98	0.42
4:H:41:GLN:OE1	4:H:59:ARG:HG3	2.19	0.42
1:A:209:LYS:HB2	2:D:294:GLU:OE1	2.20	0.42
1:B:482:LYS:NZ	1:B:496:LYS:NZ	2.67	0.42
1:C:48:GLN:HB3	2:D:68:GLY:HA2	2.02	0.42
2:D:188:GLU:O	2:D:221:GLN:HB3	2.19	0.42
2:D:247:GLU:O	2:D:249:GLN:NE2	2.52	0.42
2:E:142:LEU:HD11	2:E:370:VAL:HG12	2.02	0.42
2:E:252:LEU:HD12	2:E:254:PHE:CZ	2.54	0.42
2:D:95:MET:HE3	2:D:99:GLY:HA2	2.02	0.42
2:D:205:VAL:CG1	2:D:215:VAL:HG23	2.50	0.42
2:D:245:ASP:O	2:D:247:GLU:N	2.53	0.42
2:D:463:ILE:HD12	2:D:463:ILE:HA	1.83	0.42
3:G:179:PHE:C	3:G:181:LEU:H	2.28	0.42
5:I:4:TRP:O	5:I:7:ALA:HB3	2.20	0.42
1:C:390:MET:HE3	1:C:424:LEU:CD1	2.44	0.42
2:E:200:MET:HE2	2:E:200:MET:HA	2.01	0.42
3:G:81:ILE:HD13	3:G:171:TYR:CZ	2.55	0.42
3:G:87:LYS:HA	3:G:90:LYS:CE	2.43	0.42
3:G:128:PHE:HA	5:I:43:LYS:O	2.18	0.42
1:A:26:GLU:HA	1:A:45:ARG:HB2	2.00	0.42
2:D:170:ILE:O	2:D:174:ALA:HB3	2.20	0.42
1:B:103:LEU:HD12	1:B:121:ILE:HG21	2.02	0.42
2:E:63:MET:HE2	2:E:82:ILE:CD1	2.50	0.42
3:G:76:GLY:HA3	3:G:228:ARG:NE	2.33	0.42
4:H:38:VAL:HA	4:H:39:PRO:HD3	1.86	0.42
1:A:403:PHE:CE1	2:E:390:ILE:HD11	2.55	0.42
1:B:287:ARG:HH11	1:B:287:ARG:HD2	1.62	0.42
1:C:381:ARG:HD3	1:C:488:LYS:HZ3	1.85	0.42
2:E:199:GLU:OE2	2:E:420:VAL:HB	2.20	0.42
2:F:440:GLY:O	2:F:444:ILE:HG13	2.19	0.42
3:G:31:TYR:CD2	3:G:229:MET:HE1	2.54	0.42
3:G:74:ASP:OD1	3:G:109:GLY:HA2	2.19	0.42
1:A:261:GLY:HA2	1:A:317:GLY:O	2.21	0.41
1:C:292:GLU:O	1:C:293:ALA:HB3	2.20	0.41
1:C:360:GLY:O	1:C:429:LYS:HE2	2.20	0.41
4:H:83:THR:HB	4:H:91:GLN:HE21	1.85	0.41
5:I:5:ARG:O	5:I:7:ALA:N	2.51	0.41
1:B:460:LYS:NZ	1:B:510:ALA:HB1	2.29	0.41
1:A:439:GLU:CG	1:A:484:ARG:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:405:SER:O	2:F:409:LYS:HG3	2.20	0.41
3:G:94:ALA:C	3:G:96:LEU:H	2.28	0.41
5:I:41:THR:O	5:I:42:ILE:C	2.63	0.41
2:E:199:GLU:OE2	2:E:420:VAL:O	2.39	0.41
4:H:100:LEU:H	4:H:100:LEU:HG	1.75	0.41
2:D:162:LYS:CE	9:D:620:ALF:F4	2.58	0.41
2:F:409:LYS:HD3	2:F:457:PHE:CE1	2.56	0.41
1:B:102:GLU:HG2	1:B:122:GLY:C	2.46	0.41
1:B:180:ILE:HD12	1:B:216:LEU:HD21	2.02	0.41
1:C:409:ASP:O	1:C:410:LEU:C	2.63	0.41
3:G:51:LEU:O	3:G:55:ALA:HB3	2.20	0.41
3:G:92:GLU:O	3:G:93:ALA:C	2.63	0.41
3:G:181:LEU:HD23	3:G:184:ILE:HB	2.03	0.41
1:B:304:ARG:HH11	1:B:304:ARG:HD3	1.59	0.41
1:C:151:LYS:HE2	1:C:436:MET:SD	2.60	0.41
1:C:213:VAL:O	1:C:216:LEU:HB3	2.21	0.41
2:E:113:PHE:CD2	2:E:113:PHE:N	2.89	0.41
2:E:406:ARG:NE	2:E:445:LEU:O	2.53	0.41
2:F:246:GLN:O	2:F:247:GLU:HG2	2.21	0.41
3:G:10:LEU:HD13	3:G:246:LEU:HB3	2.02	0.41
4:H:64:VAL:HG12	4:H:72:THR:HG22	2.03	0.41
1:A:446:TYR:OH	1:A:494:ASP:OD1	2.34	0.41
1:B:452:TYR:OH	1:B:498:LYS:HG3	2.21	0.41
1:C:171:ARG:HG2	11:C:2209:HOH:O	2.21	0.41
2:D:84:ILE:HD13	2:D:235:THR:HG23	2.02	0.41
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.31	0.41
3:G:57:ILE:HG22	3:G:184:ILE:HD12	2.02	0.41
1:A:355:GLU:HB3	11:A:2220:HOH:O	2.20	0.41
1:A:484:ARG:NH2	11:A:2287:HOH:O	2.54	0.41
1:B:67:GLU:HB3	1:B:68:PRO:HD2	2.02	0.41
1:C:137:ILE:N	1:C:138:PRO:CD	2.84	0.41
1:C:163:GLN:HG3	1:C:347:ASP:HB2	2.03	0.41
2:E:122:GLU:HB2	2:E:125:GLU:HG3	2.01	0.41
2:F:442:GLN:NE2	11:F:2272:HOH:O	2.52	0.41
3:G:178:ILE:HD12	3:G:212:ILE:HG21	2.03	0.41
1:B:503:ASN:HD22	1:B:503:ASN:HA	1.61	0.40
2:D:275:ILE:HD13	2:D:275:ILE:HG21	1.89	0.40
2:D:282:GLN:HE21	2:D:282:GLN:N	1.86	0.40
3:G:197:ASP:C	3:G:199:ASP:N	2.79	0.40
1:A:48:GLN:HG2	2:E:70:VAL:CG2	2.51	0.40
2:E:176:ALA:C	2:E:178:GLY:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:LEU:HD22	2:F:441:PHE:CD1	2.57	0.40
3:G:21:LYS:HE2	3:G:236:SER:HB2	2.04	0.40
3:G:260:LYS:HB2	3:G:260:LYS:HE3	1.61	0.40
1:B:397:TYR:C	1:B:399:GLU:N	2.79	0.40
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.85	0.40
1:B:508:PHE:CE2	1:B:510:ALA:HB3	2.56	0.40
1:C:432:GLN:O	1:C:433:TYR:HB2	2.21	0.40
2:D:285:LEU:C	2:D:285:LEU:HD23	2.46	0.40
2:E:391:LEU:HD11	3:G:26:VAL:HA	2.03	0.40
2:F:126:MET:HA	2:F:126:MET:HE2	2.03	0.40
3:G:67:LEU:HA	3:G:104:LYS:O	2.20	0.40
1:A:439:GLU:HG3	1:A:484:ARG:HB2	2.04	0.40
1:B:209:LYS:HZ2	2:E:356:ARG:NH1	2.18	0.40
2:E:163:THR:O	2:E:167:MET:HG3	2.22	0.40
2:E:173:VAL:O	11:E:2078:HOH:O	2.22	0.40
2:F:244:ARG:O	2:F:248:GLY:HA2	2.21	0.40
3:G:67:LEU:N	11:G:2007:HOH:O	2.54	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	482/510 (94%)	466 (97%)	12 (2%)	4 (1%)	16	11
1	B	475/510 (93%)	456 (96%)	15 (3%)	4 (1%)	16	11
1	C	484/510 (95%)	475 (98%)	9 (2%)	0	100	100
2	D	465/482 (96%)	448 (96%)	13 (3%)	4 (1%)	14	9
2	E	450/482 (93%)	407 (90%)	31 (7%)	12 (3%)	4	1
2	F	464/482 (96%)	437 (94%)	22 (5%)	5 (1%)	11	7
3	G	234/272 (86%)	197 (84%)	29 (12%)	8 (3%)	3	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	87/146 (60%)	79 (91%)	5 (6%)	3 (3%)	3	1
5	I	32/50 (64%)	28 (88%)	2 (6%)	2 (6%)	1	0
All	All	3173/3444 (92%)	2993 (94%)	138 (4%)	42 (1%)	9	5

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	LYS
1	B	413	ALA
2	E	176	ALA
2	E	444	ILE
2	F	246	GLN
3	G	79	GLY
3	G	102	GLU
3	G	180	SER
3	G	194	ASP
3	G	195	ASP
4	H	49	ALA
1	B	194	ASP
1	B	398	ARG
2	D	246	GLN
2	D	248	GLY
2	E	28	GLY
2	E	174	ALA
2	E	365	SER
2	E	366	GLU
2	F	28	GLY
2	F	175	LYS
2	F	398	GLU
3	G	130	GLU
3	G	196	ILE
2	E	448	GLU
4	H	71	THR
1	A	20	ASP
1	A	22	SER
2	D	474	ALA
2	E	175	LYS
2	E	357	ILE
4	H	88	SER
5	I	40	SER
2	D	247	GLU

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Mol	Chain	Res	Type
2	E	177	HIS
3	G	37	GLU
2	E	456	ALA
5	I	42	ILE
1	B	458	PRO
2	E	279	VAL
1	A	489	ILE
2	F	279	VAL

5.3.2 Protein sidechains [i](#)

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%)	377 (96%)	16 (4%)	27	26
1	B	388/412 (94%)	376 (97%)	12 (3%)	35	37
1	C	394/412 (96%)	385 (98%)	9 (2%)	44	49
2	D	377/386 (98%)	366 (97%)	11 (3%)	37	40
2	E	368/386 (95%)	351 (95%)	17 (5%)	24	22
2	F	376/386 (97%)	361 (96%)	15 (4%)	28	27
3	G	207/230 (90%)	194 (94%)	13 (6%)	16	13
4	H	75/109 (69%)	68 (91%)	7 (9%)	8	5
5	I	29/41 (71%)	25 (86%)	4 (14%)	3	2
All	All	2607/2774 (94%)	2503 (96%)	104 (4%)	28	27

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	25	LEU
1	A	80	LYS
1	A	123	SER
1	A	157	VAL
1	A	188	ARG

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Mol	Chain	Res	Type
1	A	216	LEU
1	A	218	LYS
1	A	384	LYS
1	A	410	LEU
1	A	414	THR
1	A	439	GLU
1	A	455	LYS
1	A	479	LEU
1	A	485	THR
1	A	494	ASP
1	B	34	ILE
1	B	87	ILE
1	B	123	SER
1	B	171	ARG
1	B	349	GLN
1	B	414	THR
1	B	416	GLN
1	B	419	SER
1	B	423	ARG
1	B	470	SER
1	B	479	LEU
1	B	497	LEU
1	C	59	LEU
1	C	121	ILE
1	C	216	LEU
1	C	219	ARG
1	C	349	GLN
1	C	384	LYS
1	C	422	VAL
1	C	457	GLU
1	C	479	LEU
2	D	56	SER
2	D	74	LYS
2	D	129	GLU
2	D	223	ASN
2	D	237	LEU
2	D	266	SER
2	D	279	VAL
2	D	282	GLN
2	D	303	SER
2	D	428	LEU
2	D	431	LEU

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Mol	Chain	Res	Type
2	E	95	MET
2	E	132	ILE
2	E	177	HIS
2	E	209	LYS
2	E	214	LYS
2	E	223	ASN
2	E	251	VAL
2	E	252	LEU
2	E	258	ILE
2	E	282	GLN
2	E	310	ILE
2	E	344	ILE
2	E	359	ASP
2	E	383	SER
2	E	431	LEU
2	E	436	GLU
2	E	452	LEU
2	F	17	ILE
2	F	95	MET
2	F	166	ILE
2	F	205	VAL
2	F	209	LYS
2	F	221	GLN
2	F	223	ASN
2	F	237	LEU
2	F	279	VAL
2	F	282	GLN
2	F	357	ILE
2	F	395	GLU
2	F	397	SER
2	F	439	LYS
2	F	455	GLN
3	G	2	THR
3	G	12	SER
3	G	15	ASN
3	G	16	ILE
3	G	77	LEU
3	G	81	ILE
3	G	91	SER
3	G	114	SER
3	G	142	SER
3	G	159	SER

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Mol	Chain	Res	Type
3	G	184	ILE
3	G	190	MET
3	G	219	GLU
4	H	33	VAL
4	H	64	VAL
4	H	68	GLU
4	H	73	SER
4	H	79	SER
4	H	91	GLN
4	H	100	LEU
5	I	17	ILE
5	I	37	THR
5	I	42	ILE
5	I	47	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	B	48	GLN
1	B	65	ASN
1	B	78	ASN
1	B	260	ASN
1	B	330	GLN
1	B	466	ASN
1	B	475	GLN
1	B	503	ASN
1	C	263	HIS
1	C	349	GLN
1	C	416	GLN
2	D	130	GLN
2	D	177	HIS
2	D	221	GLN
2	D	223	ASN
2	D	282	GLN
2	D	385	GLN
2	E	24	GLN
2	E	34	ASN
2	E	39	GLN
2	E	51	GLN
2	E	194	ASN
2	E	223	ASN

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Mol	Chain	Res	Type
2	E	263	GLN
2	E	282	GLN
2	E	293	GLN
2	E	308	GLN
2	E	361	ASN
2	F	194	ASN
2	F	198	HIS
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	379	GLN
2	F	427	HIS
2	F	442	GLN
3	G	82	HIS
3	G	88	GLN
3	G	205	GLN
4	H	91	GLN
5	I	16	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 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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$
6	ADP	A	600	7	28,29,29	1.13	3 (10%)	43,45,45	0.75	1 (2%)
6	ADP	E	600	7	28,29,29	1.03	1 (3%)	43,45,45	0.67	1 (2%)
6	ADP	D	600	7,9	28,29,29	1.22	2 (7%)	43,45,45	0.69	1 (2%)
10	SO4	E	630	-	4,4,4	0.68	0	6,6,6	0.55	0
6	ADP	F	600	7,9	28,29,29	1.02	2 (7%)	43,45,45	0.80	3 (6%)
9	ALF	D	620	6,2,7,11	4,4,4	1.39	0	-	-	-
9	ALF	F	620	6,7,11	4,4,4	1.42	0	-	-	-
8	GOL	B	700	-	5,5,5	0.40	0	5,5,5	0.56	0
8	GOL	C	602	-	5,5,5	0.32	0	5,5,5	0.81	0
8	GOL	B	602	-	5,5,5	1.02	0	5,5,5	1.91	3 (60%)
6	ADP	C	600	7	28,29,29	1.27	4 (14%)	43,45,45	0.99	5 (11%)
8	GOL	A	602	-	5,5,5	0.40	0	5,5,5	0.52	0
6	ADP	B	600	7	28,29,29	0.91	1 (3%)	43,45,45	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	A	600	7	-	2/16/32/32	0/3/3/3
6	ADP	E	600	7	-	2/16/32/32	0/3/3/3
6	ADP	D	600	7,9	-	2/16/32/32	0/3/3/3
6	ADP	F	600	7,9	-	0/16/32/32	0/3/3/3
8	GOL	B	700	-	-	2/4/4/4	-
8	GOL	C	602	-	-	3/4/4/4	-
8	GOL	B	602	-	-	2/4/4/4	-
6	ADP	C	600	7	-	2/16/32/32	0/3/3/3
8	GOL	A	602	-	-	2/4/4/4	-
6	ADP	B	600	7	-	1/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	600	ADP	PA-O3A	4.04	1.63	1.59
6	C	600	ADP	PA-O3A	3.23	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	600	ADP	PA-O3A	3.13	1.62	1.59
6	C	600	ADP	PB-O2B	-2.84	1.44	1.54
6	A	600	ADP	C2-N3	-2.69	1.29	1.33
6	F	600	ADP	PB-O2B	-2.53	1.45	1.54
6	D	600	ADP	PB-O2B	-2.43	1.45	1.54
6	C	600	ADP	PA-O2A	-2.42	1.44	1.55
6	F	600	ADP	PA-O1A	-2.35	1.42	1.50
6	C	600	ADP	C2-N1	2.20	1.37	1.33
6	B	600	ADP	PB-O3B	-2.12	1.46	1.54
6	A	600	ADP	PB-O3B	-2.07	1.47	1.54
6	A	600	ADP	C2-N1	2.04	1.37	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	602	GOL	C3-C2-C1	2.82	122.12	111.80
6	C	600	ADP	O2A-PA-O3A	2.61	114.32	107.27
8	B	602	GOL	O2-C2-C1	2.38	119.03	109.18
6	F	600	ADP	O3B-PB-O2B	2.38	116.72	107.80
6	E	600	ADP	O2B-PB-O3A	2.21	112.03	104.64
6	A	600	ADP	O3B-PB-O1B	2.20	119.41	110.83
6	C	600	ADP	C1'-N9-C8	2.20	131.97	127.09
6	C	600	ADP	O2B-PB-O3A	2.17	111.91	104.64
6	C	600	ADP	O3B-PB-O3A	-2.16	97.39	104.64
8	B	602	GOL	O2-C2-C3	2.15	118.06	109.18
6	D	600	ADP	O3A-PA-O1A	2.10	117.02	110.70
6	F	600	ADP	O5'-PA-O1A	2.07	117.12	108.94
6	F	600	ADP	O4'-C4'-C3'	-2.06	101.07	105.15
6	C	600	ADP	C4-N9-C1'	-2.05	121.84	126.63

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	600	ADP	PA-O3A-PB-O2B
6	C	600	ADP	PA-O3A-PB-O2B
6	D	600	ADP	PA-O3A-PB-O2B
6	D	600	ADP	PA-O3A-PB-O3B
6	E	600	ADP	PA-O3A-PB-O2B
8	B	700	GOL	C1-C2-C3-O3
8	C	602	GOL	O1-C1-C2-C3
8	A	602	GOL	C1-C2-C3-O3

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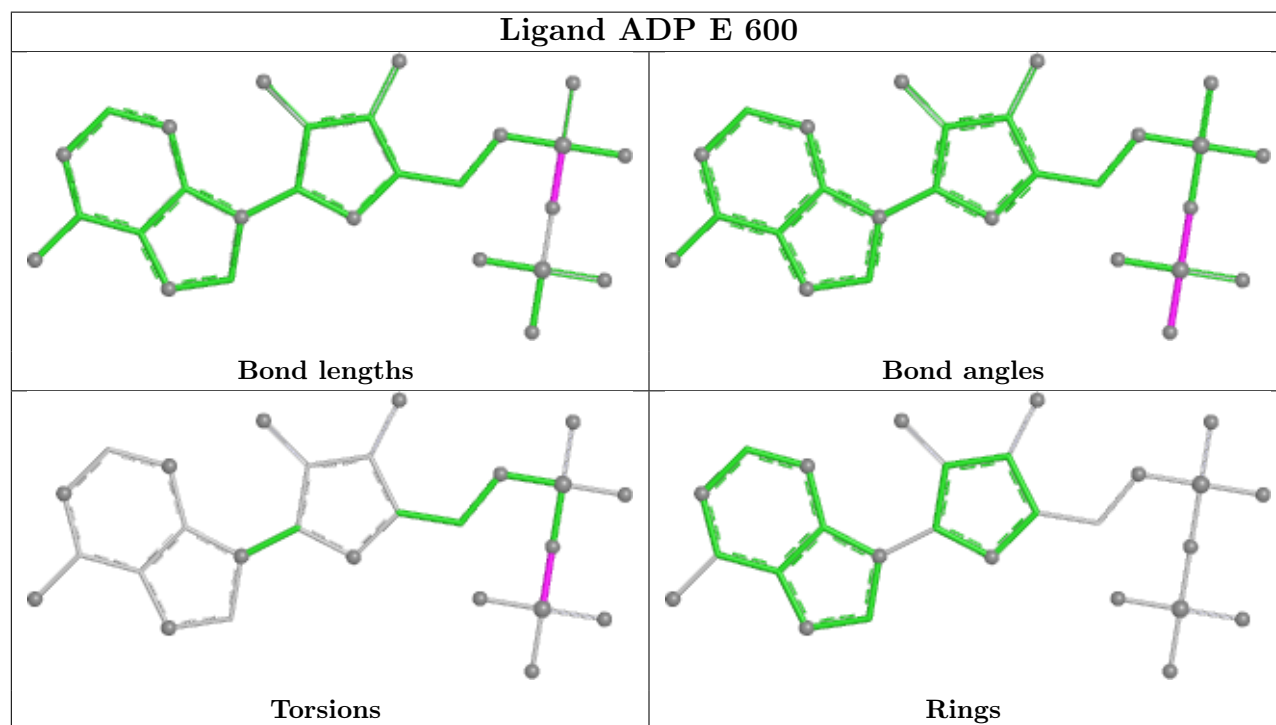
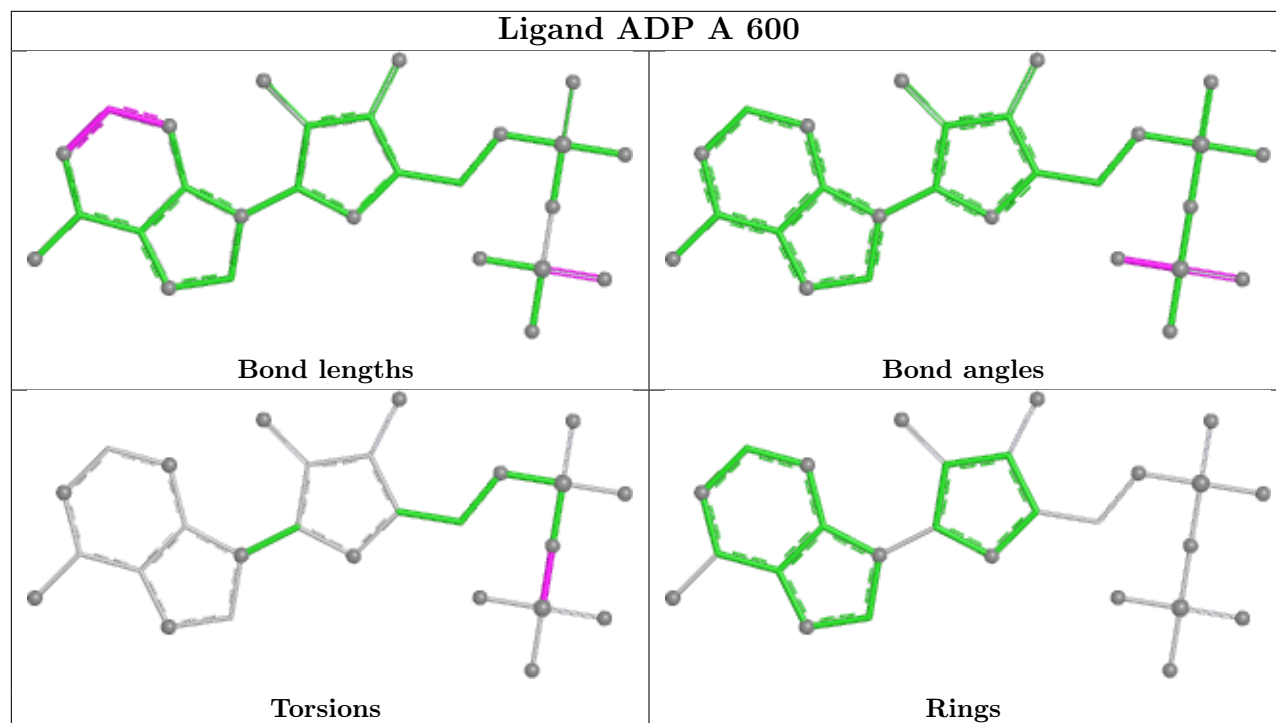
Mol	Chain	Res	Type	Atoms
8	B	602	GOL	C1-C2-C3-O3
8	B	700	GOL	O2-C2-C3-O3
8	B	602	GOL	O1-C1-C2-O2
8	C	602	GOL	O1-C1-C2-O2
6	A	600	ADP	PA-O3A-PB-O1B
8	C	602	GOL	O2-C2-C3-O3
6	C	600	ADP	PA-O3A-PB-O1B
8	A	602	GOL	O2-C2-C3-O3
6	B	600	ADP	PA-O3A-PB-O1B
6	E	600	ADP	PA-O3A-PB-O1B

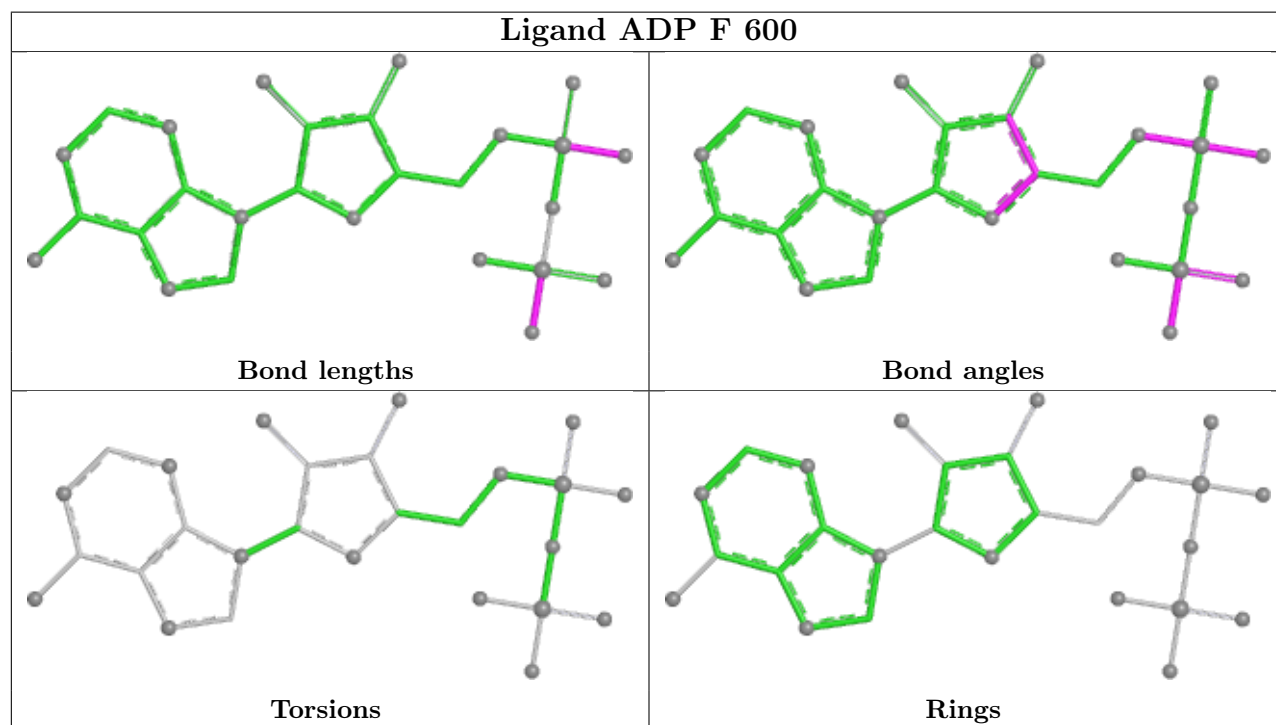
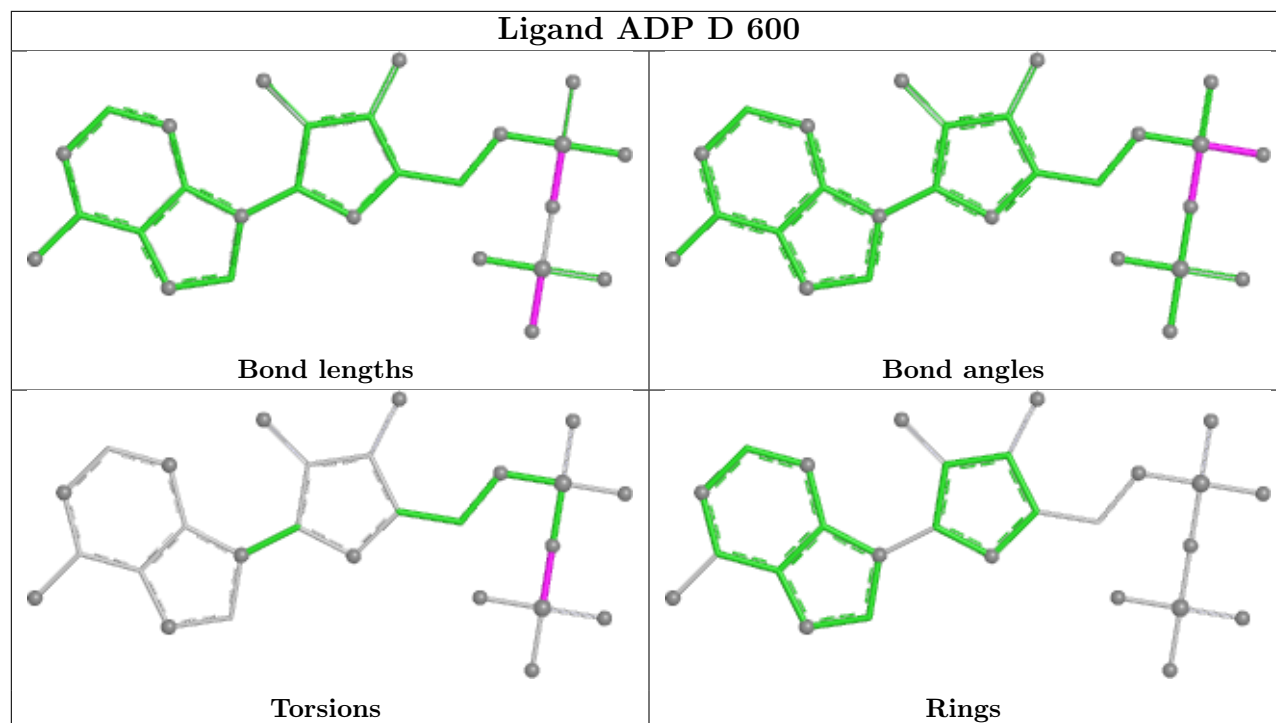
There are no ring outliers.

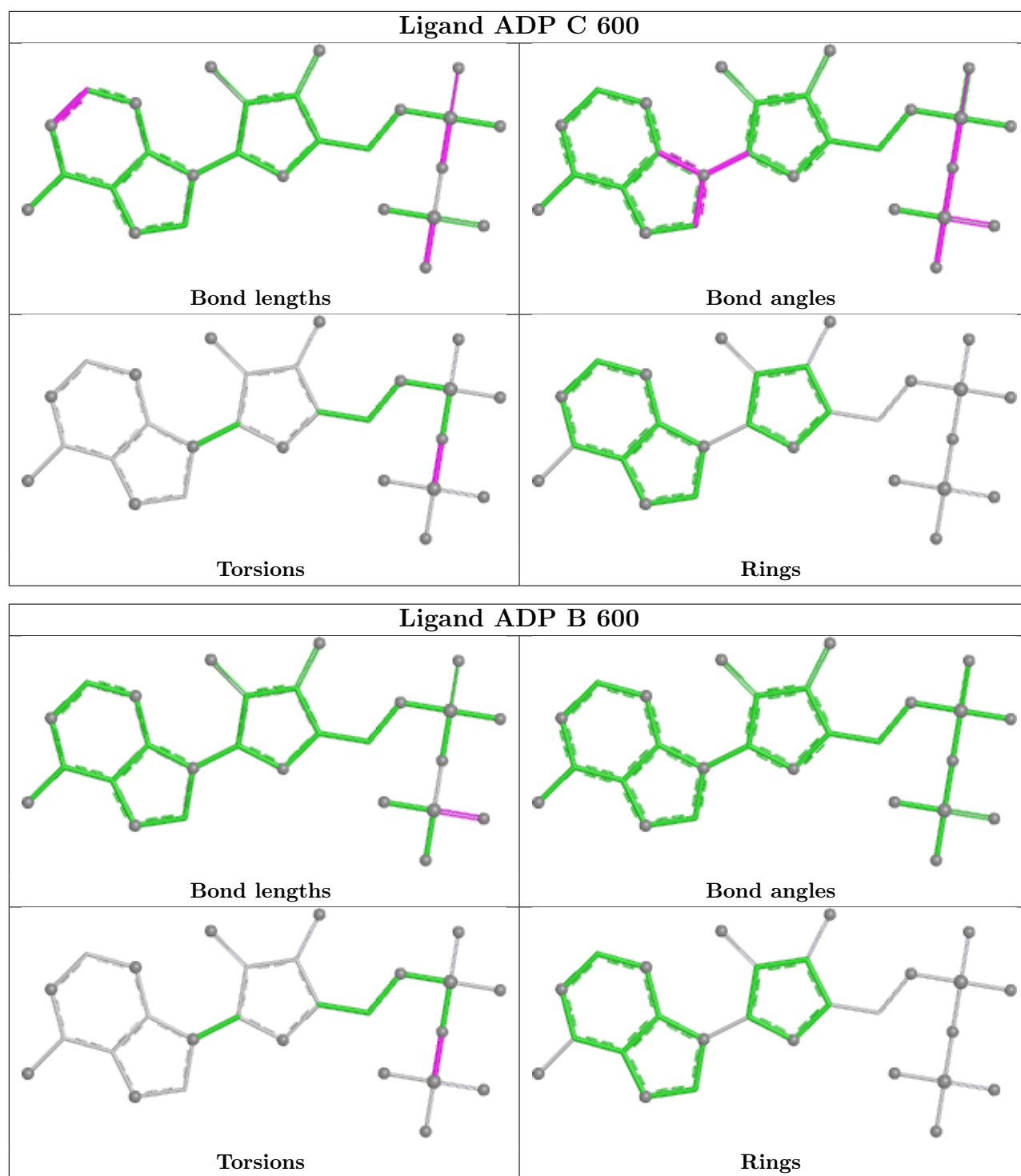
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	620	ALF	3	0
8	B	700	GOL	1	0
8	C	602	GOL	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	486/510 (95%)	-0.27	5 (1%) 79 79	24, 36, 57, 98	0
1	B	479/510 (93%)	-0.04	13 (2%) 56 55	24, 38, 71, 113	0
1	C	488/510 (95%)	-0.40	3 (0%) 85 85	22, 34, 53, 82	0
2	D	467/482 (96%)	-0.36	7 (1%) 72 71	24, 34, 57, 83	0
2	E	454/482 (94%)	0.61	66 (14%) 6 5	24, 47, 105, 120	0
2	F	466/482 (96%)	-0.21	16 (3%) 48 47	23, 34, 65, 88	0
3	G	244/272 (89%)	1.41	68 (27%) 1 1	28, 66, 95, 115	0
4	H	89/146 (60%)	1.61	27 (30%) 1 1	51, 73, 110, 122	0
5	I	36/50 (72%)	2.90	28 (77%) 0 0	58, 87, 113, 119	0
All	All	3209/3444 (93%)	0.08	233 (7%) 21 19	22, 38, 86, 122	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	7	ALA	7.8
2	E	456	ALA	7.0
3	G	180	SER	6.8
1	A	402	ALA	6.7
2	E	444	ILE	5.8
1	A	19	ALA	5.7
2	E	178	GLY	5.6
3	G	181	LEU	5.6
5	I	25	ALA	5.5
5	I	47	VAL	5.5
3	G	165	PHE	5.0
2	F	474	ALA	4.9
2	F	174	ALA	4.8
2	E	446	ALA	4.8
2	E	364	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
2	E	402	LEU	4.7
2	E	452	LEU	4.7
2	E	174	ALA	4.5
1	A	403	PHE	4.5
4	H	71	THR	4.5
1	B	400	VAL	4.5
2	E	176	ALA	4.4
2	F	248	GLY	4.3
3	G	27	ALA	4.3
3	G	198	ALA	4.3
4	H	67	ALA	4.3
1	B	414	THR	4.3
4	H	72	THR	4.3
3	G	55	ALA	4.3
4	H	33	VAL	4.2
2	E	368	TYR	4.2
2	E	371	ALA	4.1
5	I	39	GLY	4.1
2	E	360	PRO	4.1
3	G	113	ARG	4.0
1	B	410	LEU	4.0
3	G	117	HIS	4.0
3	G	199	ASP	4.0
2	F	246	GLN	3.9
2	E	370	VAL	3.9
2	E	449	TYR	3.9
5	I	12	ILE	3.9
2	E	357	ILE	3.8
1	C	409	ASP	3.8
1	B	358	TYR	3.8
4	H	44	ALA	3.7
2	E	445	LEU	3.7
3	G	103	VAL	3.7
5	I	42	ILE	3.7
2	E	356	ARG	3.7
2	E	453	PRO	3.6
5	I	3	TYR	3.6
1	B	413	ALA	3.6
4	H	43	GLY	3.6
2	F	397	SER	3.6
5	I	22	VAL	3.5
2	F	388	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
3	G	96	LEU	3.5
2	E	355	SER	3.5
4	H	77	VAL	3.5
3	G	150	ASN	3.5
3	G	187	ALA	3.5
2	E	384	LEU	3.5
3	G	57	ILE	3.4
5	I	19	ALA	3.4
2	E	387	ILE	3.4
3	G	196	ILE	3.4
2	E	391	LEU	3.3
4	H	103	LEU	3.3
3	G	54	LYS	3.3
2	E	362	ILE	3.3
2	F	391	LEU	3.3
1	A	20	ASP	3.3
5	I	37	THR	3.3
3	G	182	ASP	3.3
2	E	432	VAL	3.2
5	I	43	LYS	3.2
2	D	386	ASP	3.2
3	G	200	VAL	3.2
1	B	510	ALA	3.2
3	G	80	ALA	3.2
2	E	396	LEU	3.2
5	I	21	ALA	3.2
5	I	44	ILE	3.1
5	I	40	SER	3.1
2	E	363	VAL	3.1
2	E	454	GLU	3.1
2	F	387	ILE	3.0
3	G	178	ILE	3.0
3	G	186	SER	3.0
2	D	475	GLU	3.0
2	E	177	HIS	3.0
3	G	195	ASP	3.0
3	G	138	PHE	3.0
2	E	366	GLU	3.0
3	G	183	THR	3.0
3	G	39	LYS	3.0
3	G	223	SER	2.9
3	G	116	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	367	HIS	2.9
5	I	6	GLN	2.9
3	G	179	PHE	2.9
4	H	45	PHE	2.9
5	I	14	TYR	2.9
3	G	92	GLU	2.9
2	D	248	GLY	2.9
5	I	38	SER	2.9
2	E	373	GLY	2.9
2	E	372	ARG	2.9
2	E	354	THR	2.8
4	H	68	GLU	2.8
2	D	178	GLY	2.8
3	G	132	GLY	2.8
3	G	26	VAL	2.8
5	I	1	VAL	2.8
3	G	105	ILE	2.8
2	F	249	GLN	2.8
2	E	393	MET	2.8
2	E	179	GLY	2.8
3	G	107	GLY	2.8
4	H	48	LEU	2.8
2	D	397	SER	2.8
2	F	175	LYS	2.8
2	E	460	VAL	2.8
3	G	111	LYS	2.7
4	H	100	LEU	2.7
2	E	439	LYS	2.7
3	G	173	THR	2.7
5	I	41	THR	2.7
4	H	26	VAL	2.7
5	I	18	CYS	2.7
5	I	2	ALA	2.7
3	G	149	LEU	2.7
2	E	427	HIS	2.7
1	B	401	ALA	2.6
4	H	70	GLY	2.6
3	G	88	GLN	2.6
5	I	4	TRP	2.6
2	F	177	HIS	2.6
3	G	77	LEU	2.6
2	F	386	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	G	68	ILE	2.6
5	I	17	ILE	2.6
1	B	412	ALA	2.6
2	E	407	ALA	2.6
3	G	134	ARG	2.6
3	G	221	THR	2.6
2	E	450	ASP	2.6
2	E	457	PHE	2.5
2	E	209	LYS	2.5
5	I	24	ASP	2.5
3	G	81	ILE	2.5
4	H	64	VAL	2.5
2	E	361	ASN	2.5
1	B	416	GLN	2.5
2	D	176	ALA	2.5
2	E	369	ASP	2.5
2	E	448	GLU	2.5
2	E	435	LYS	2.5
3	G	70	GLY	2.5
3	G	168	VAL	2.4
2	F	398	GLU	2.4
3	G	114	SER	2.4
2	E	358	MET	2.4
2	E	451	HIS	2.4
3	G	115	ILE	2.4
3	G	83	SER	2.4
4	H	31	ALA	2.4
2	E	426	GLY	2.4
2	D	387	ILE	2.4
3	G	192	ILE	2.4
2	E	175	LYS	2.4
3	G	8	ARG	2.4
3	G	166	ARG	2.4
2	E	405	SER	2.4
1	C	19	ALA	2.3
2	E	211	ALA	2.3
1	B	392	LEU	2.3
3	G	15	ASN	2.3
2	E	447	GLY	2.3
2	E	148	LYS	2.3
5	I	5	ARG	2.3
3	G	69	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
3	G	137	THR	2.3
1	C	23	VAL	2.3
3	G	33	ARG	2.3
2	E	386	ASP	2.3
3	G	94	ALA	2.3
2	F	392	GLY	2.3
3	G	170	SER	2.2
4	H	47	ILE	2.2
2	F	396	LEU	2.2
2	E	9	THR	2.2
3	G	112	ILE	2.2
4	H	65	VAL	2.2
3	G	50	ALA	2.2
2	E	431	LEU	2.2
5	I	15	SER	2.2
4	H	42	THR	2.2
3	G	71	VAL	2.2
2	E	429	GLY	2.2
1	B	411	ASP	2.2
2	E	428	LEU	2.1
3	G	248	LEU	2.1
4	H	99	THR	2.1
3	G	131	VAL	2.1
2	E	401	LYS	2.1
3	G	25	MET	2.1
2	E	359	ASP	2.1
2	F	250	ASP	2.1
3	G	5	ASP	2.1
4	H	87	ASP	2.1
3	G	31	TYR	2.1
2	E	437	THR	2.1
1	A	487	GLY	2.1
5	I	23	ARG	2.1
2	E	374	VAL	2.1
3	G	1	ALA	2.1
3	G	201	LEU	2.1
4	H	32	ASN	2.1
3	G	127	THR	2.1
3	G	108	VAL	2.1
4	H	27	PHE	2.1
1	B	419	SER	2.1
2	E	353	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	365	SER	2.1
4	H	73	SER	2.1
1	B	482	LYS	2.0
2	E	131	GLU	2.0
5	I	45	VAL	2.0
4	H	69	ASP	2.0
4	H	34	ARG	2.0
4	H	59	ARG	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.

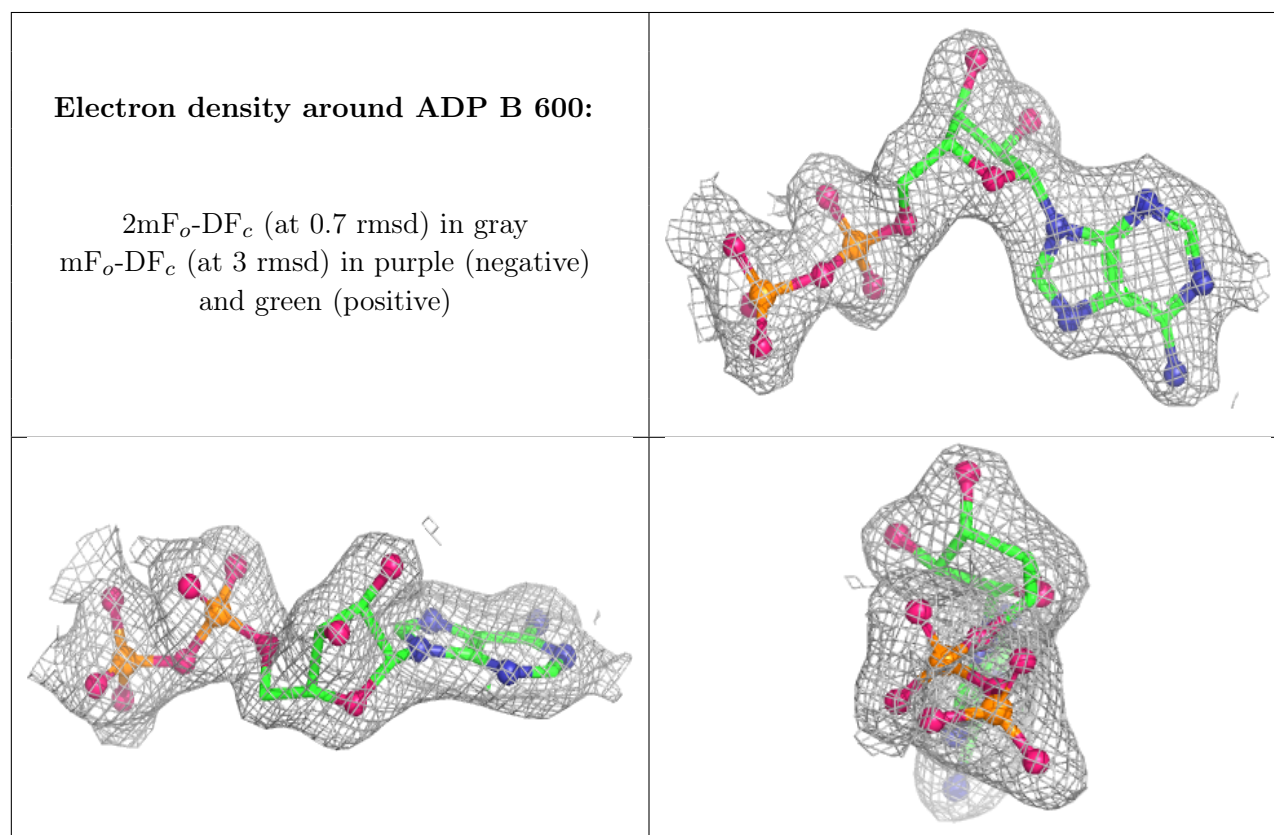
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	B	700	6/6	0.73	0.18	67,71,72,73	0
8	GOL	A	602	6/6	0.90	0.08	42,42,44,46	0
9	ALF	D	620	5/5	0.90	0.13	37,37,40,41	0
8	GOL	C	602	6/6	0.95	0.06	33,34,36,37	0
7	MG	C	601	1/1	0.95	0.05	30,30,30,30	0
10	SO4	E	630	5/5	0.95	0.11	36,40,41,44	0
8	GOL	B	602	6/6	0.97	0.05	31,35,36,39	0
6	ADP	B	600	27/27	0.97	0.06	30,39,42,45	0
7	MG	E	601	1/1	0.97	0.06	42,42,42,42	0
7	MG	F	601	1/1	0.97	0.03	28,28,28,28	0
9	ALF	F	620	5/5	0.97	0.07	33,33,34,35	0
6	ADP	E	600	27/27	0.97	0.07	35,42,46,47	0
6	ADP	C	600	27/27	0.98	0.06	25,29,31,33	0
6	ADP	A	600	27/27	0.98	0.05	25,34,37,44	0
7	MG	A	601	1/1	0.99	0.04	33,33,33,33	0

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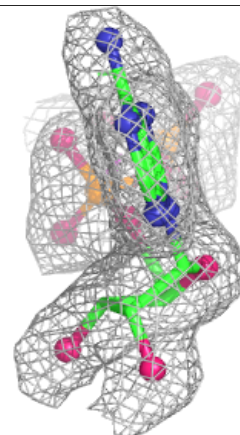
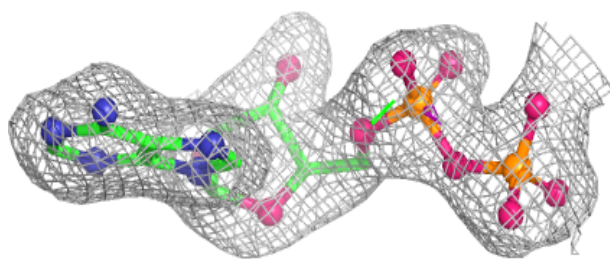
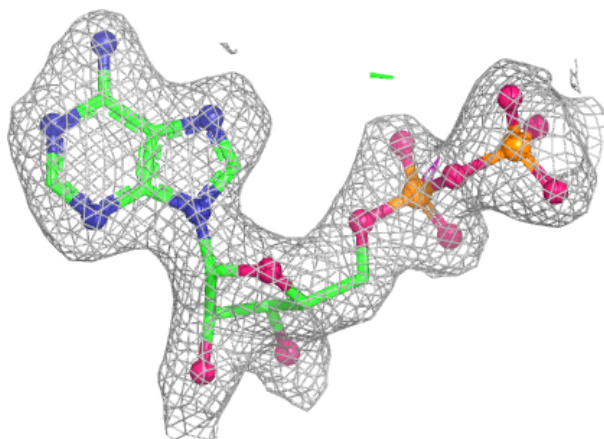
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	B	601	1/1	0.99	0.02	35,35,35,35	0
6	ADP	D	600	27/27	0.99	0.04	24,27,30,31	0
6	ADP	F	600	27/27	0.99	0.04	24,30,34,36	0
7	MG	D	601	1/1	1.00	0.03	30,30,30,30	0

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.

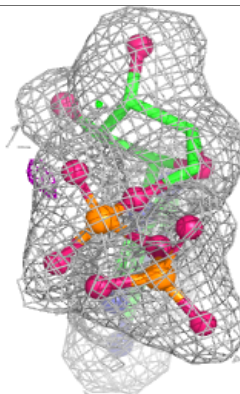
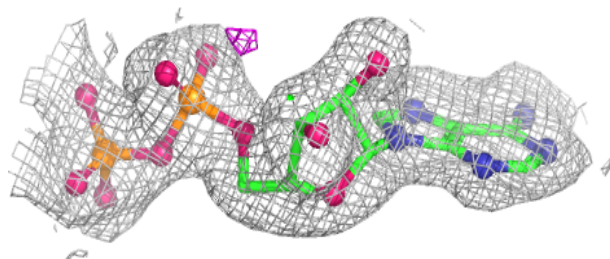
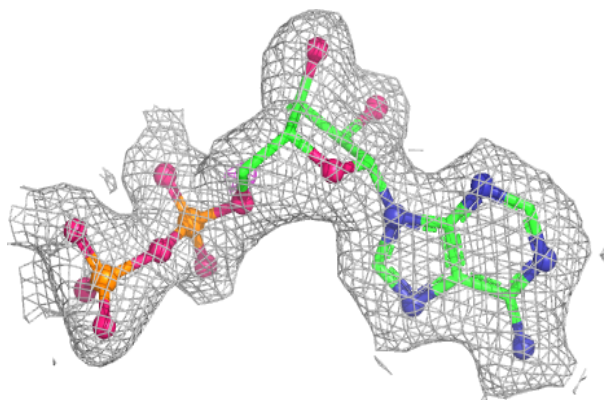


Electron density around ADP E 600:

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

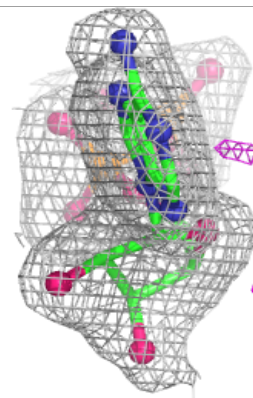
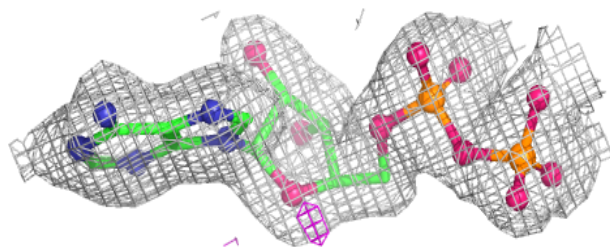
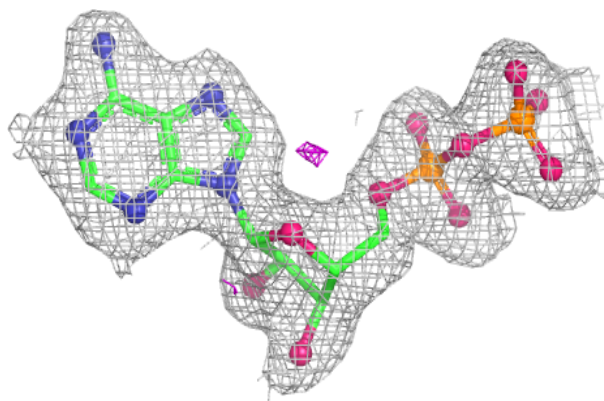
**Electron density around ADP C 600:**

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

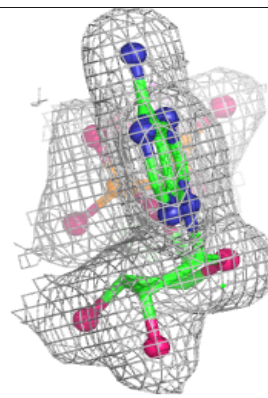
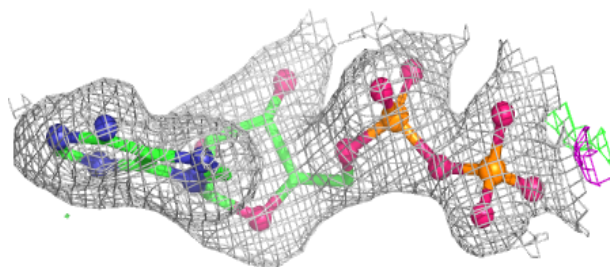
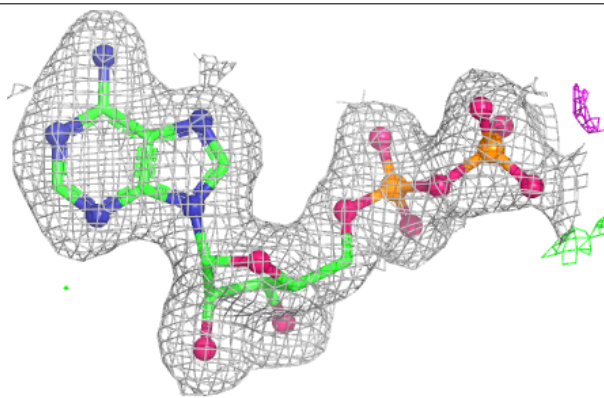


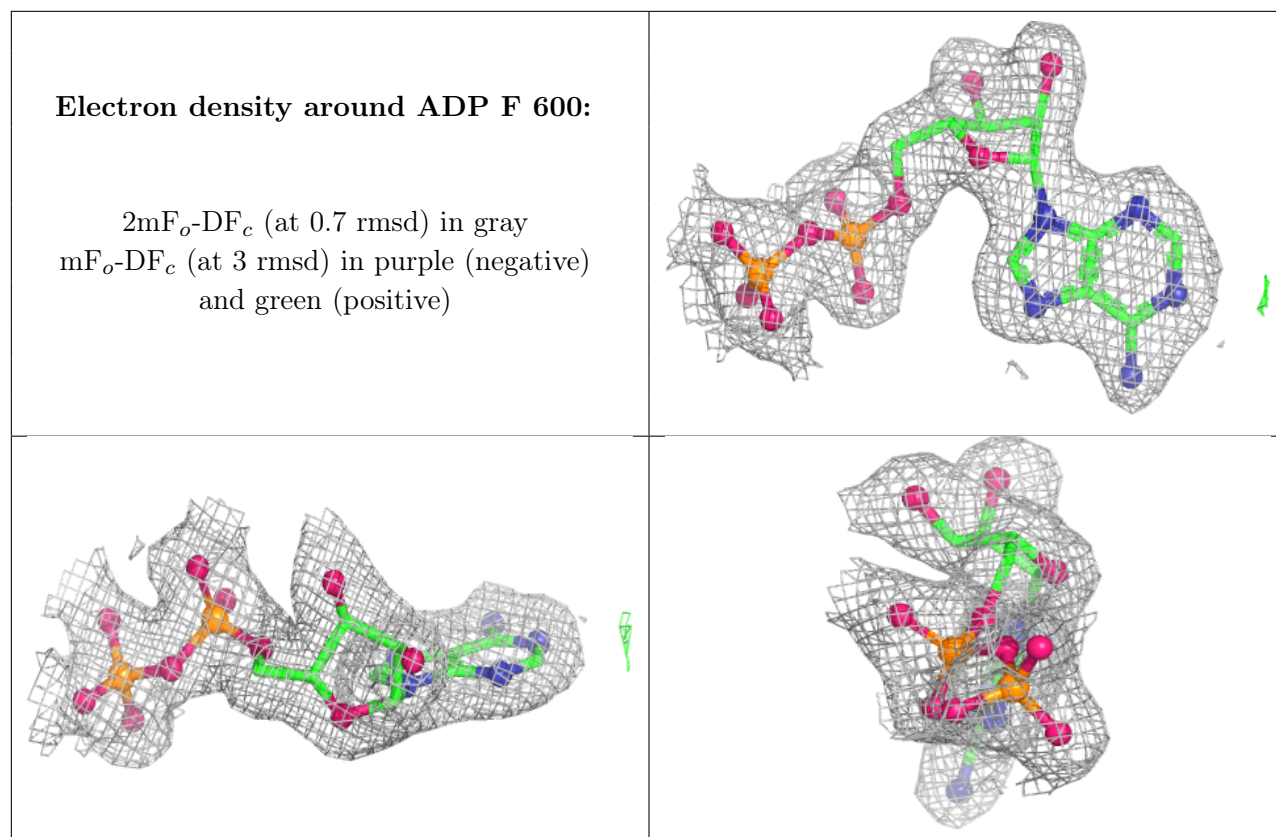
Electron density around ADP A 600:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.