



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:19 AM UTC

PDB ID : 1E79 / pdb_00001e79
Title : Bovine F1-ATPase inhibited by DCCD (dicyclohexylcarbodiimide)
Authors : Gibbons, C.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2000-08-25
Resolution : 2.40 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

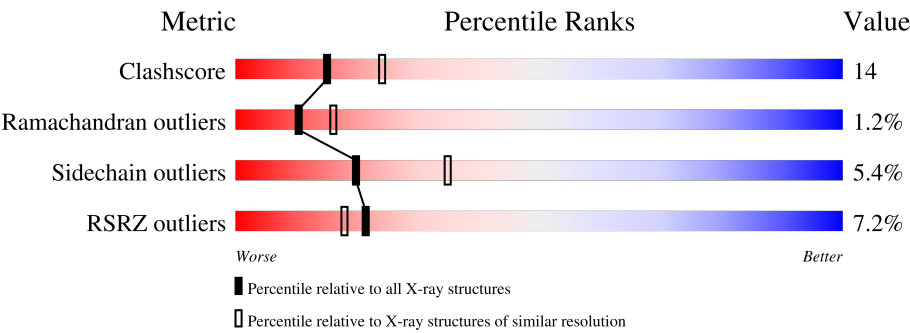
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	510	2% 73% 21% . .
1	B	510	7% 68% 23% 5% . . .
1	C	510	% 74% 20% . .
2	D	482	% 74% 21% . .
2	E	482	7% 70% 22% . . .
2	F	482	2% 73% 21% . .

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Mol	Chain	Length	Quality of chain
3	G	272	20% 58% 31% 7%
4	H	146	40% 48% 36% 5% 10%
5	I	50	46% 56% 28% 8% 6%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26318 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 ATP SYNTHASE ALPHA CHAIN HEART ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			
1	B	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	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	cloning artifact	UNP P19483
B	481	GLY	SER	cloning artifact	UNP P19483
C	481	GLY	SER	cloning artifact	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3538	2243	601	683	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 ATP SYNTHASE GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	263	Total	C	N	O	S	0	0	0
			2051	1291	354	398	8			

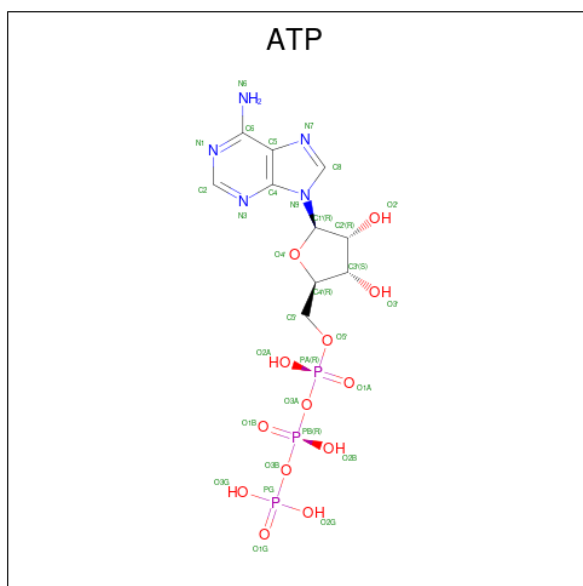
- Molecule 4 is a protein called ATP SYNTHASE DELTA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	131	Total	C	N	O	S	0	0	0
			970	609	164	195	2			

- Molecule 5 is a protein called ATP SYNTHASE EPSILON CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	47	Total	C	N	O	S	0	0	0
			369	237	66	64	2			

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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

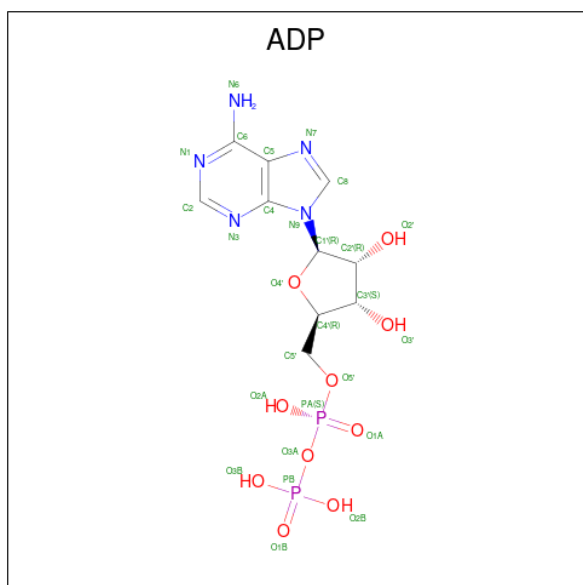
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

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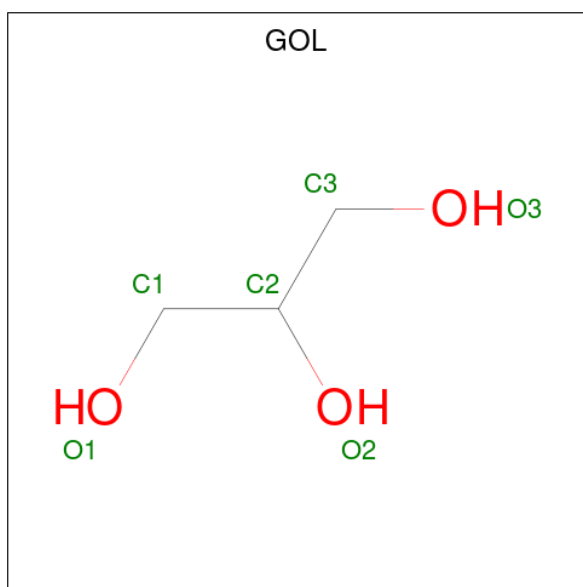
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



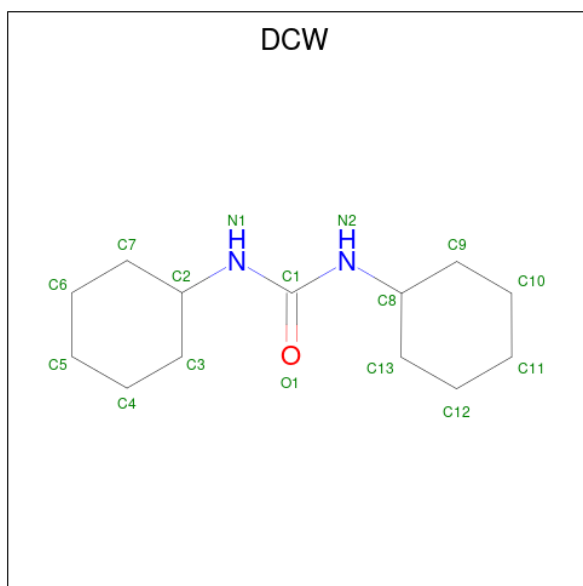
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



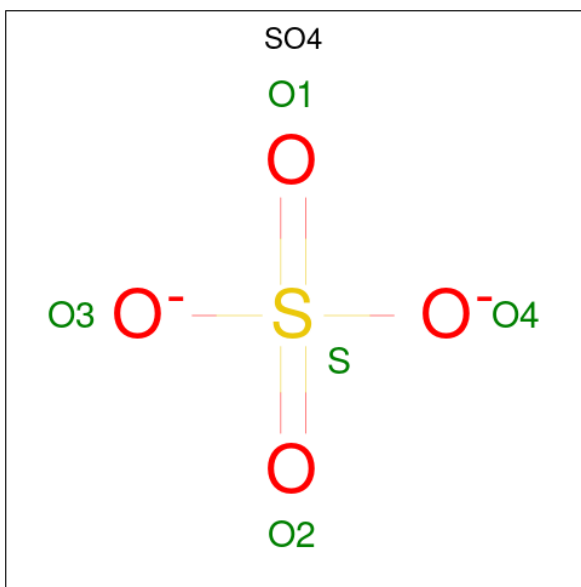
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is DICYCLOHEXYLUREA (CCD ID: DCW) (formula: $C_{13}H_{24}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			16	13	2	1		

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

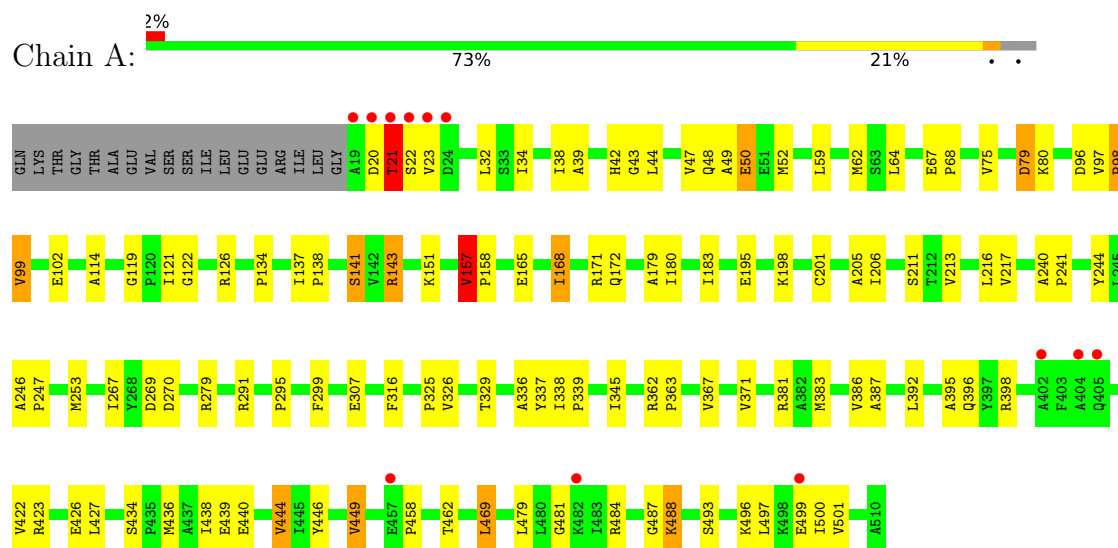
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	163	Total	O	0	0
			163	163		
12	B	140	Total	O	0	0
			140	140		
12	C	167	Total	O	0	0
			167	167		
12	D	148	Total	O	0	0
			148	148		
12	E	95	Total	O	0	0
			95	95		
12	F	164	Total	O	0	0
			164	164		
12	G	25	Total	O	0	0
			25	25		
12	H	5	Total	O	0	0
			5	5		
12	I	4	Total	O	0	0
			4	4		

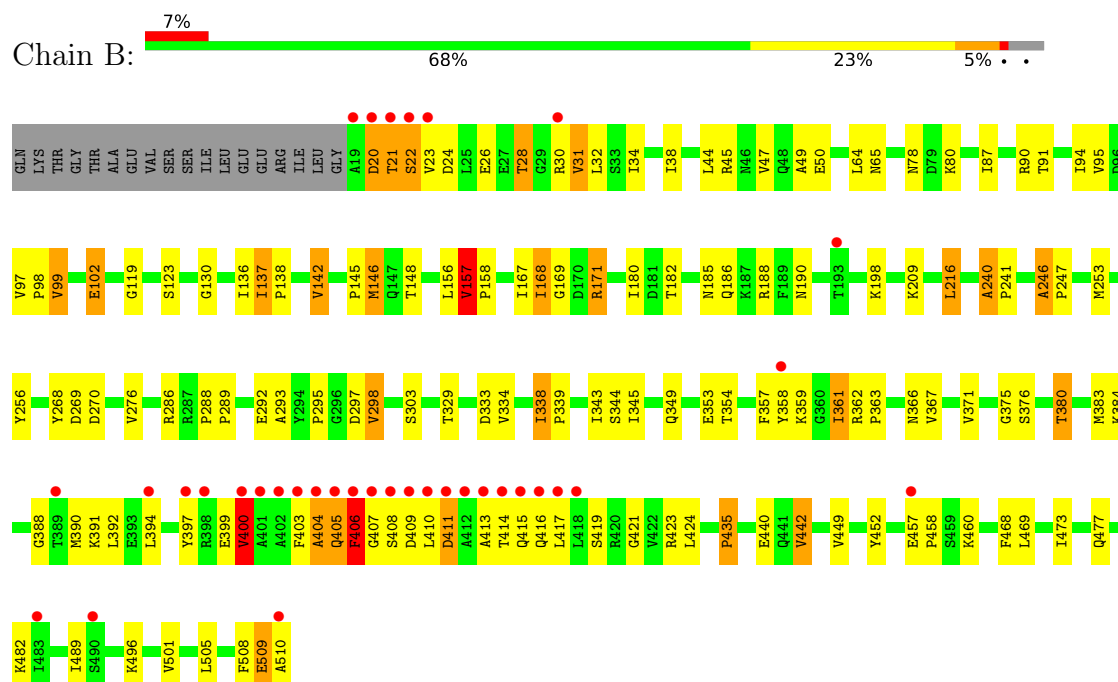
3 Residue-property plots [i](#)

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

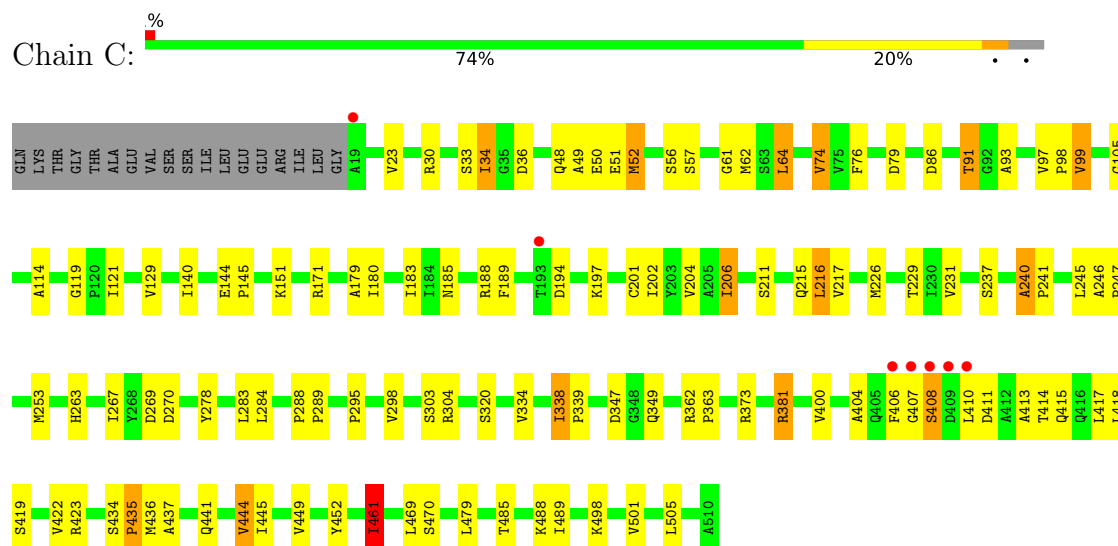
• Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM



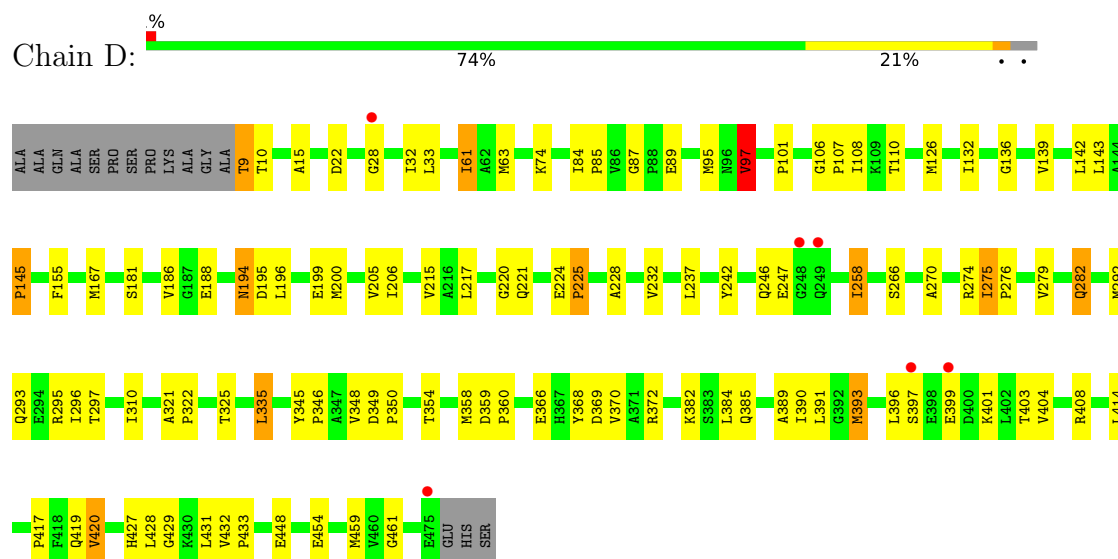
• Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM



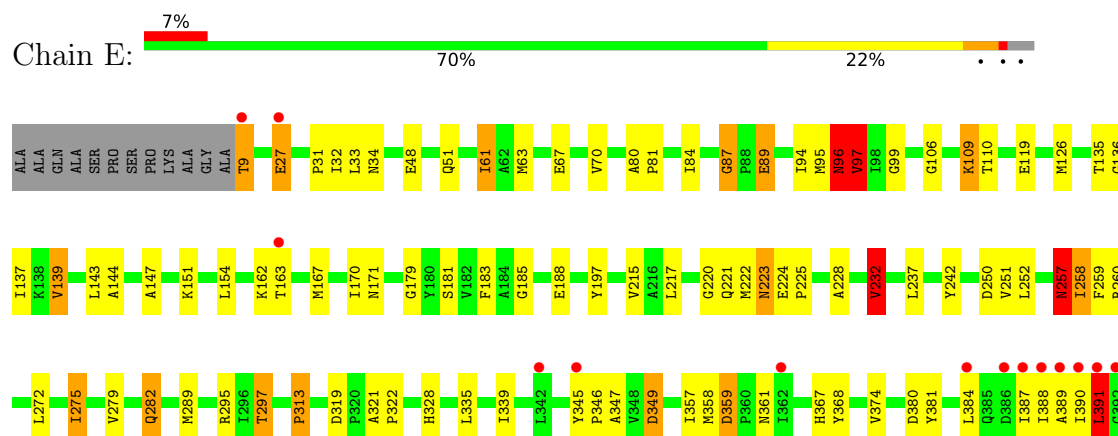
• Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM

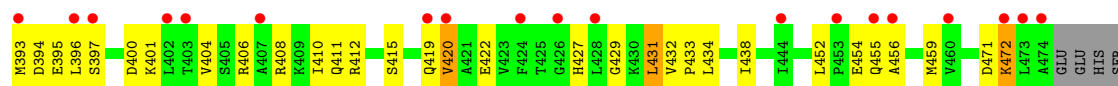


• Molecule 2: ATP SYNTHASE BETA CHAIN

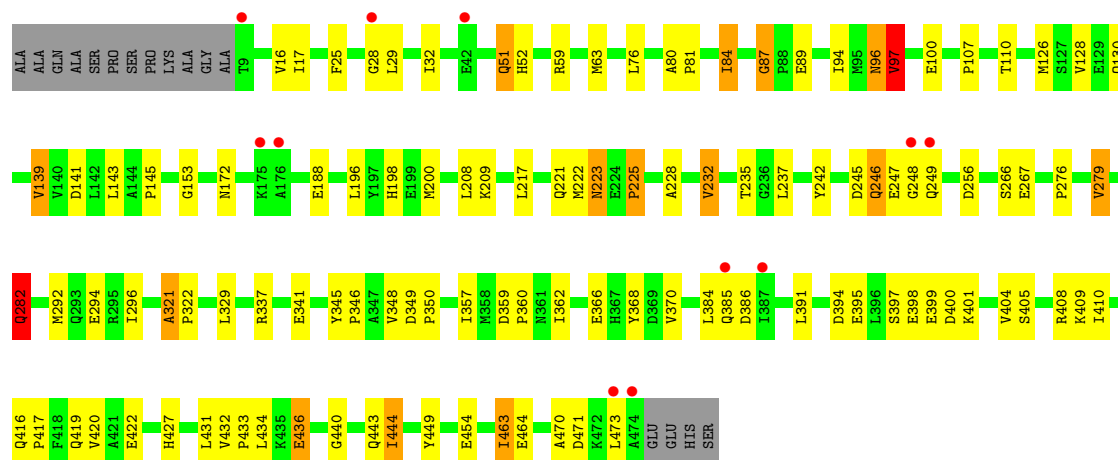


• Molecule 2: ATP SYNTHASE BETA CHAIN

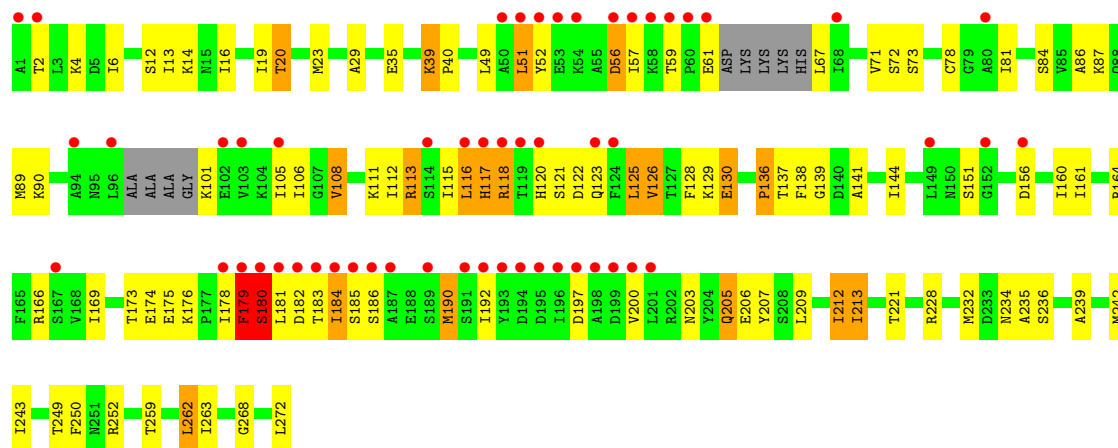




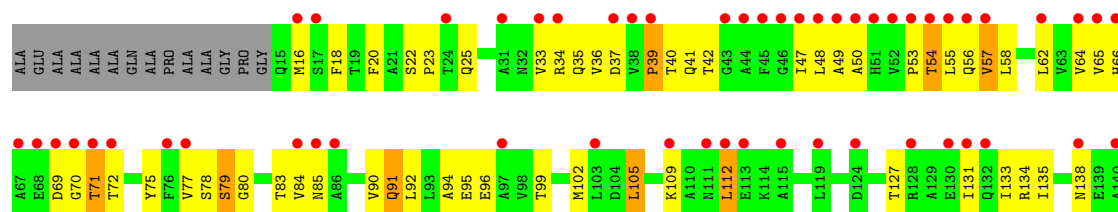
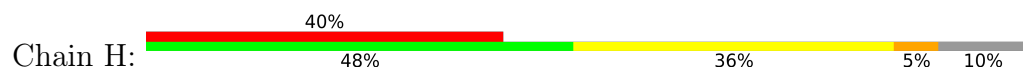
• Molecule 2: ATP SYNTHASE BETA CHAIN

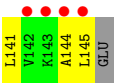


• Molecule 3: ATP SYNTHASE GAMMA CHAIN

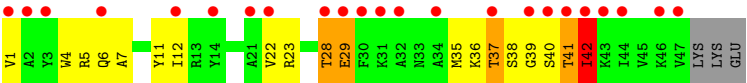


• Molecule 4: ATP SYNTHASE DELTA CHAIN





● Molecule 5: ATP SYNTHASE EPSILON CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	267.20Å 107.20Å 135.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.2 (20.00-2.40) 91.7 (20.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.281 0.204 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26318	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: ATP, ADP, MG, GOL, DCW, 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	0.47	0/3799	1.13	10/5126 (0.2%)
1	B	0.50	0/3799	1.17	28/5126 (0.5%)
1	C	0.49	0/3799	1.15	10/5126 (0.2%)
2	D	0.50	1/3595 (0.0%)	1.18	21/4877 (0.4%)
2	E	0.47	0/3587	1.13	26/4867 (0.5%)
2	F	0.48	0/3587	1.16	22/4867 (0.5%)
3	G	0.45	0/2074	1.02	5/2785 (0.2%)
4	H	0.41	0/982	0.99	2/1337 (0.1%)
5	I	0.44	0/374	0.96	0/501
All	All	0.48	1/25596 (0.0%)	1.13	124/34612 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	195	ASP	N-CA	-6.62	1.38	1.46

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	195	ASP	N-CA-CB	11.16	126.21	109.91
1	B	23	VAL	N-CA-C	8.64	121.86	109.51
1	B	22	SER	CA-C-N	8.55	132.28	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	SER	C-N-CA	8.55	132.28	120.49
2	E	97	VAL	CB-CA-C	-8.01	101.55	112.04
2	D	97	VAL	CB-CA-C	-7.95	101.62	112.04
4	H	39	PRO	N-CA-CB	7.86	107.32	102.92
2	E	257	ASN	CA-CB-CG	7.56	120.16	112.60
2	F	139	VAL	CB-CA-C	-7.42	102.48	111.97
2	F	225	PRO	CA-C-N	7.12	126.65	119.24
2	F	225	PRO	C-N-CA	7.12	126.65	119.24
3	G	179	PHE	CA-CB-CG	7.11	120.91	113.80
2	F	198	HIS	CA-CB-CG	-7.09	106.71	113.80
2	D	194	ASN	CA-C-N	6.79	129.62	120.65
2	D	194	ASN	C-N-CA	6.79	129.62	120.65
1	B	20	ASP	CA-CB-CG	6.68	119.28	112.60
4	H	69	ASP	N-CA-C	6.58	118.55	109.54
1	B	137	ILE	CA-C-N	6.53	126.22	119.82
1	B	137	ILE	C-N-CA	6.53	126.22	119.82
2	F	143	LEU	N-CA-C	6.42	119.59	111.69
1	A	79	ASP	CA-CB-CG	6.35	118.95	112.60
1	C	303	SER	CA-C-N	6.31	129.06	120.54
1	C	303	SER	C-N-CA	6.31	129.06	120.54
1	C	338	ILE	CA-C-N	6.30	125.52	118.97
1	C	338	ILE	C-N-CA	6.30	125.52	118.97
2	E	275	ILE	CA-C-N	6.21	126.13	119.85
2	E	275	ILE	C-N-CA	6.21	126.13	119.85
1	B	136	ILE	N-CA-C	6.14	116.31	110.42
2	D	275	ILE	N-CA-C	-6.06	103.42	108.63
2	D	225	PRO	CA-C-N	6.04	125.75	119.05
2	D	225	PRO	C-N-CA	6.04	125.75	119.05
1	B	145	PRO	N-CA-CB	5.97	108.55	103.35
2	F	321	ALA	CA-C-N	5.92	125.13	118.97
2	F	321	ALA	C-N-CA	5.92	125.13	118.97
2	D	61	ILE	N-CA-CB	5.88	119.52	111.41
1	B	21	THR	N-CA-C	-5.87	103.92	113.19
2	E	144	ALA	CA-C-N	5.86	125.80	119.76
2	E	144	ALA	C-N-CA	5.86	125.80	119.76
1	C	461	ILE	N-CA-C	5.82	116.55	110.62
1	B	246	ALA	CA-C-N	5.81	125.01	118.97
1	B	246	ALA	C-N-CA	5.81	125.01	118.97
2	E	139	VAL	CB-CA-C	-5.80	104.45	111.88
2	E	225	PRO	CA-C-N	5.79	125.92	119.32
2	E	225	PRO	C-N-CA	5.79	125.92	119.32
2	D	275	ILE	CB-CA-C	-5.74	105.60	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	ILE	CA-C-N	5.74	125.42	119.05
1	B	338	ILE	C-N-CA	5.74	125.42	119.05
1	A	75	VAL	N-CA-C	5.73	116.83	108.58
1	B	20	ASP	CA-C-N	5.68	130.50	121.18
1	B	20	ASP	C-N-CA	5.68	130.50	121.18
2	D	106	GLY	CA-C-N	5.67	125.69	119.90
2	D	106	GLY	C-N-CA	5.67	125.69	119.90
2	E	143	LEU	N-CA-C	5.67	119.37	112.23
1	B	91	THR	N-CA-C	-5.65	106.74	113.97
1	C	119	GLY	CA-C-N	5.63	125.56	119.76
1	C	119	GLY	C-N-CA	5.63	125.56	119.76
1	A	157	VAL	CA-C-N	5.62	125.90	119.83
1	A	157	VAL	C-N-CA	5.62	125.90	119.83
2	E	433	PRO	N-CA-CB	5.53	108.23	103.31
2	D	359	ASP	CA-CB-CG	5.53	118.12	112.60
2	E	359	ASP	CA-C-N	5.45	125.53	119.32
2	E	359	ASP	C-N-CA	5.45	125.53	119.32
1	B	20	ASP	N-CA-CB	5.43	118.12	110.36
1	A	134	PRO	N-CA-CB	5.42	108.02	103.25
2	F	256	ASP	CA-CB-CG	5.41	118.01	112.60
2	D	432	VAL	N-CA-C	5.41	113.90	107.73
2	E	349	ASP	CA-C-N	5.41	125.02	119.56
2	E	349	ASP	C-N-CA	5.41	125.02	119.56
1	A	137	ILE	N-CA-C	5.39	120.52	108.88
1	B	38	ILE	N-CA-C	5.37	116.32	108.53
1	A	337	TYR	N-CA-C	5.37	116.82	110.97
2	F	97	VAL	CB-CA-C	-5.35	102.51	111.29
3	G	39	LYS	CA-C-N	5.33	124.52	118.97
3	G	39	LYS	C-N-CA	5.33	124.52	118.97
2	F	87	GLY	CA-C-N	5.33	125.00	119.56
2	F	87	GLY	C-N-CA	5.33	125.00	119.56
1	A	119	GLY	CA-C-N	5.33	125.25	119.76
1	A	119	GLY	C-N-CA	5.33	125.25	119.76
2	F	84	ILE	CA-C-N	5.33	125.09	119.76
2	F	84	ILE	C-N-CA	5.33	125.09	119.76
1	B	435	PRO	N-CA-CB	5.32	108.04	103.31
2	E	432	VAL	N-CA-C	5.30	113.11	107.76
2	D	461	GLY	CA-C-N	5.27	125.25	120.03
2	D	461	GLY	C-N-CA	5.27	125.25	120.03
2	D	349	ASP	CA-C-N	5.23	124.84	119.56
2	D	349	ASP	C-N-CA	5.23	124.84	119.56
2	E	106	GLY	CA-C-N	5.20	125.14	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	106	GLY	C-N-CA	5.20	125.14	119.78
2	D	107	PRO	N-CA-CB	5.19	107.81	103.25
1	B	157	VAL	CA-C-N	5.17	125.41	119.83
1	B	157	VAL	C-N-CA	5.17	125.41	119.83
2	D	427	HIS	CA-CB-CG	5.16	118.96	113.80
2	E	313	PRO	N-CA-CB	5.15	107.83	103.19
2	F	282	GLN	CA-C-N	5.15	124.76	119.56
2	F	282	GLN	C-N-CA	5.15	124.76	119.56
1	B	119	GLY	CA-C-N	5.15	125.08	119.78
1	B	119	GLY	C-N-CA	5.15	125.08	119.78
2	E	87	GLY	CA-C-N	5.14	125.44	119.47
2	E	87	GLY	C-N-CA	5.14	125.44	119.47
1	B	288	PRO	CA-C-N	5.14	124.90	119.76
1	B	288	PRO	C-N-CA	5.14	124.90	119.76
2	F	349	ASP	CA-C-N	5.13	124.74	119.56
2	F	349	ASP	C-N-CA	5.13	124.74	119.56
1	A	98	PRO	N-CA-CB	5.12	107.81	103.35
2	F	145	PRO	N-CA-CB	5.12	107.86	103.31
3	G	136	PRO	N-CA-CB	5.11	107.80	103.35
3	G	117	HIS	CA-CB-CG	-5.10	108.70	113.80
2	E	96	ASN	CA-CB-CG	5.10	117.70	112.60
2	F	107	PRO	N-CA-CB	5.08	107.83	103.31
2	E	452	LEU	CA-C-N	5.07	125.47	119.99
2	E	452	LEU	C-N-CA	5.07	125.47	119.99
2	F	276	PRO	N-CA-CB	5.07	107.76	103.35
1	B	137	ILE	N-CA-C	5.06	118.42	112.35
2	E	232	VAL	N-CA-CB	5.04	116.77	110.47
1	C	240	ALA	CA-C-N	5.03	124.81	119.28
1	C	240	ALA	C-N-CA	5.03	124.81	119.28
2	D	145	PRO	N-CA-CB	5.03	107.78	103.31
2	F	359	ASP	CA-C-N	5.02	125.04	119.32
2	F	359	ASP	C-N-CA	5.02	125.04	119.32
1	B	240	ALA	CA-C-N	5.01	124.61	119.05
1	B	240	ALA	C-N-CA	5.01	124.61	119.05
2	D	433	PRO	N-CA-CB	5.01	107.71	103.35
2	E	139	VAL	N-CA-CB	5.01	116.07	110.51
1	C	435	PRO	N-CA-CB	5.00	107.76	103.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	194	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	3748	0	3844	81	0
1	B	3748	0	3844	111	0
1	C	3748	0	3844	79	0
2	D	3538	0	3592	95	0
2	E	3530	0	3587	98	0
2	F	3530	0	3586	94	0
3	G	2051	0	2115	113	0
4	H	970	0	972	59	0
5	I	369	0	395	21	0
6	A	31	0	12	0	0
6	C	31	0	12	1	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	F	1	0	0	0	0
8	B	27	0	12	0	0
8	D	27	0	12	0	0
8	F	27	0	12	0	0
9	B	6	0	8	1	0
10	D	16	0	23	6	0
11	E	5	0	0	0	0
12	A	163	0	0	4	0
12	B	140	0	0	3	0
12	C	167	0	0	2	0
12	D	148	0	0	10	0
12	E	95	0	0	0	0
12	F	164	0	0	5	0
12	G	25	0	0	1	0
12	H	5	0	0	0	0
12	I	4	0	0	0	0
All	All	26318	0	25870	702	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 (702) 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:D:199:GLU:HG2	10:D:700:DCW:H71C	1.32	1.08
2:D:199:GLU:CG	10:D:700:DCW:H71C	1.85	1.06
3:G:90:LYS:HB3	3:G:116:LEU:HD11	1.38	1.01
1:B:406:PHE:HB2	1:B:409:ASP:HB2	1.44	1.00
1:A:211:SER:HB3	2:D:126:MET:HE2	1.43	1.00
2:F:282:GLN:H	2:F:282:GLN:HE21	1.00	0.98
2:E:181:SER:HB2	2:E:215:VAL:HG12	1.45	0.96
1:C:211:SER:HB3	2:F:126:MET:HE2	1.46	0.95
3:G:19:ILE:HG22	3:G:23:MET:HE2	1.49	0.95
4:H:62:LEU:HD11	4:H:144:ALA:HB2	1.49	0.92
2:E:282:GLN:H	2:E:282:GLN:HE21	1.16	0.91
2:E:257:ASN:HD21	2:E:259:PHE:HB3	1.35	0.91
4:H:85:ASN:HD21	4:H:91:GLN:HE22	1.13	0.90
2:F:196:LEU:HD11	2:F:200:MET:HE3	1.50	0.89
2:D:282:GLN:H	2:D:282:GLN:HE21	0.91	0.88
3:G:20:THR:HG22	3:G:236:SER:HB3	1.57	0.87
2:D:282:GLN:H	2:D:282:GLN:NE2	1.71	0.86
2:F:282:GLN:H	2:F:282:GLN:NE2	1.77	0.81
4:H:105:LEU:HD22	4:H:109:LYS:HE3	1.63	0.81
1:B:47:VAL:HG12	1:B:90:ARG:HG2	1.62	0.81
3:G:161:ILE:HG12	3:G:175:GLU:HG2	1.63	0.81
3:G:89:MET:HE1	3:G:112:ILE:HG23	1.63	0.80
3:G:89:MET:HB3	3:G:116:LEU:HD22	1.63	0.80
2:E:388:ILE:HG12	2:E:396:LEU:HD11	1.62	0.80
3:G:178:ILE:HG22	3:G:180:SER:HB2	1.65	0.79
2:D:275:ILE:HD13	3:G:272:LEU:HD12	1.64	0.79
3:G:121:SER:C	3:G:123:GLN:H	1.91	0.79
3:G:137:THR:HG21	5:I:39:GLY:H	1.48	0.78
2:D:167:MET:HE1	2:D:196:LEU:HD22	1.65	0.77
2:D:282:GLN:HE21	2:D:282:GLN:N	1.76	0.77
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.68	0.76
3:G:117:HIS:ND1	3:G:118:ARG:N	2.34	0.76
2:D:10:THR:HG21	2:D:74:LYS:HE3	1.68	0.75
1:B:97:VAL:HB	1:B:98:PRO:HD2	1.68	0.75
3:G:86:ALA:HA	3:G:89:MET:HE3	1.67	0.74
4:H:138:ASN:HA	4:H:141:LEU:HD12	1.68	0.74
1:C:423:ARG:HD2	1:C:461:ILE:HD11	1.70	0.74

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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	0.73
4:H:34:ARG:HH22	4:H:70:GLY:HA2	1.52	0.73
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.70	0.73
4:H:85:ASN:HD21	4:H:91:GLN:NE2	1.87	0.72
2:F:89:GLU:HB2	2:F:110:THR:HG22	1.71	0.72
1:C:183:ILE:HD12	1:C:201:CYS:HB3	1.69	0.72
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.71	0.72
3:G:57:ILE:CG2	3:G:184:ILE:HD12	2.19	0.72
1:B:406:PHE:CE1	1:B:410:LEU:HB2	2.25	0.72
4:H:84:VAL:HG12	4:H:90:VAL:HG22	1.72	0.72
1:C:179:ALA:HB1	1:C:267:ILE:HD13	1.71	0.71
2:D:89:GLU:HG3	2:D:110:THR:HA	1.71	0.71
2:E:390:ILE:O	2:E:391:LEU:HB2	1.90	0.71
4:H:133:ILE:HD11	5:I:4:TRP:HB3	1.73	0.71
1:A:246:ALA:HB3	1:A:247:PRO:HD3	1.72	0.70
5:I:35:MET:C	5:I:37:THR:H	1.99	0.70
1:A:383:MET:HE2	1:A:387:ALA:HB2	1.72	0.69
1:B:102:GLU:HG3	1:B:123:SER:HA	1.74	0.69
1:B:343:ILE:HD12	1:B:349:GLN:HG2	1.75	0.69
1:B:246:ALA:HB3	1:B:247:PRO:HD3	1.74	0.68
2:F:471:ASP:C	2:F:473:LEU:H	2.01	0.68
3:G:115:ILE:C	3:G:117:HIS:H	2.01	0.68
1:C:52:MET:HE1	1:C:76:PHE:CE2	2.29	0.68
2:E:170:ILE:HD13	2:E:215:VAL:HG11	1.75	0.67
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.77	0.67
3:G:137:THR:HG22	3:G:139:GLY:H	1.60	0.67
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.75	0.67
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.76	0.67
1:B:289:PRO:HG2	3:G:263:ILE:HD12	1.76	0.67
3:G:14:LYS:HG3	3:G:243:ILE:HD12	1.76	0.67
1:A:141:SER:O	1:A:143:ARG:HD3	1.95	0.67
4:H:65:VAL:C	4:H:72:THR:HG23	2.19	0.67
1:B:30:ARG:NH1	1:B:32:LEU:HD23	2.10	0.67
3:G:178:ILE:C	3:G:180:SER:H	2.04	0.66
2:E:282:GLN:H	2:E:282:GLN:NE2	1.92	0.66
2:E:408:ARG:O	2:E:412:ARG:HG2	1.94	0.66
2:F:444:ILE:HD11	2:F:463:ILE:HD11	1.78	0.66
2:F:410:ILE:HG13	2:F:444:ILE:HG21	1.78	0.66
1:A:362:ARG:HA	1:A:363:PRO:C	2.21	0.66
2:E:9:THR:HG21	2:E:27:GLU:HG3	1.78	0.66
2:F:208:LEU:O	2:F:209:LYS:HE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:185:GLY:HA3	2:E:188:GLU:HG2	1.79	0.65
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.79	0.65
2:F:440:GLY:O	2:F:444:ILE:HD13	1.97	0.65
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.62	0.64
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.79	0.64
4:H:54:THR:N	4:H:84:VAL:HG23	2.13	0.64
3:G:39:LYS:HB3	3:G:40:PRO:HD3	1.80	0.63
1:B:168:ILE:HD11	1:B:329:THR:CG2	2.28	0.63
2:F:172:ASN:ND2	2:F:431:LEU:HD11	2.14	0.63
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.80	0.63
5:I:5:ARG:C	5:I:7:ALA:H	2.06	0.63
3:G:141:ALA:HB1	3:G:213:ILE:HG23	1.81	0.63
2:F:63:MET:CE	2:F:228:ALA:HA	2.29	0.63
1:C:52:MET:HE1	1:C:76:PHE:HE2	1.62	0.63
1:A:179:ALA:HB1	1:A:267:ILE:HD13	1.79	0.63
2:D:139:VAL:HA	12:D:2048:HOH:O	1.99	0.63
1:B:410:LEU:HD21	1:B:414:THR:HB	1.80	0.63
3:G:61:GLU:OE1	3:G:101:LYS:HG2	1.99	0.62
2:D:258:ILE:HD11	2:D:292:MET:SD	2.39	0.62
1:B:362:ARG:HA	1:B:363:PRO:C	2.23	0.62
2:D:101:PRO:HB3	2:D:108:ILE:HD11	1.81	0.62
4:H:54:THR:H	4:H:84:VAL:HG23	1.65	0.62
1:C:97:VAL:HB	1:C:98:PRO:HD2	1.82	0.61
1:A:180:ILE:CD1	1:A:216:LEU:HD21	2.30	0.61
1:B:80:LYS:HD2	2:E:33:LEU:HD12	1.82	0.61
1:C:91:THR:HG23	1:C:93:ALA:H	1.65	0.61
1:C:211:SER:CB	2:F:126:MET:HE2	2.28	0.61
2:D:321:ALA:HB3	2:D:322:PRO:HD3	1.83	0.61
3:G:184:ILE:C	3:G:186:SER:H	2.08	0.61
1:B:30:ARG:O	1:B:31:VAL:HB	2.01	0.61
2:D:143:LEU:HG	12:D:2048:HOH:O	2.00	0.61
1:C:362:ARG:HA	1:C:363:PRO:C	2.26	0.60
2:D:136:GLY:HA3	2:D:431:LEU:CD1	2.32	0.60
2:E:147:ALA:HB2	2:E:357:ILE:HD13	1.82	0.60
1:A:183:ILE:HD12	1:A:201:CYS:HB3	1.83	0.60
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.84	0.60
1:B:44:LEU:HB3	1:B:47:VAL:HG13	1.83	0.60
2:D:393:MET:HG3	2:D:396:LEU:HD12	1.84	0.60
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.84	0.59
1:B:338:ILE:HB	1:B:339:PRO:HD3	1.84	0.59
1:B:20:ASP:HB3	1:B:22:SER:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:VAL:HG21	1:B:489:ILE:HD11	1.84	0.59
2:F:126:MET:HE3	12:F:2052:HOH:O	2.02	0.59
3:G:57:ILE:CG2	3:G:184:ILE:CD1	2.81	0.59
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.84	0.59
4:H:37:ASP:HB2	4:H:64:VAL:HB	1.85	0.59
2:F:419:GLN:NE2	2:F:431:LEU:HD13	2.17	0.59
1:C:91:THR:CG2	1:C:93:ALA:H	2.16	0.59
2:F:471:ASP:C	2:F:473:LEU:N	2.61	0.59
1:C:381:ARG:H	1:C:381:ARG:HD2	1.68	0.59
3:G:207:TYR:HA	5:I:12:ILE:HD11	1.84	0.59
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.83	0.58
1:A:151:LYS:HD3	1:A:436:MET:SD	2.43	0.58
2:E:390:ILE:CG2	3:G:29:ALA:HB2	2.33	0.58
3:G:156:ASP:HA	3:G:181:LEU:HD13	1.85	0.58
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.84	0.58
2:D:419:GLN:HA	2:D:429:GLY:HA3	1.85	0.58
2:E:404:VAL:O	2:E:408:ARG:HG3	2.03	0.58
1:A:44:LEU:O	1:A:47:VAL:HG22	2.04	0.58
3:G:87:LYS:O	3:G:90:LYS:HG2	2.04	0.58
4:H:64:VAL:HG13	4:H:72:THR:HG21	1.85	0.58
3:G:180:SER:O	3:G:205:GLN:HG3	2.04	0.58
1:C:347:ASP:C	1:C:373:ARG:HG3	2.28	0.57
1:B:146:MET:HE1	1:B:186:GLN:NE2	2.19	0.57
2:D:199:GLU:CG	10:D:700:DCW:C7	2.63	0.57
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.33	0.57
2:F:419:GLN:HE21	2:F:431:LEU:HD13	1.67	0.57
4:H:96:GLU:OE2	5:I:23:ARG:NE	2.38	0.57
2:F:245:ASP:C	2:F:247:GLU:H	2.11	0.57
3:G:57:ILE:HG23	3:G:184:ILE:CD1	2.35	0.57
3:G:164:ARG:NH2	3:G:166:ARG:HD3	2.20	0.57
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.70	0.57
2:F:32:ILE:HD12	2:F:51:GLN:HA	1.86	0.56
1:A:96:ASP:OD1	1:A:126:ARG:NH1	2.38	0.56
1:A:499:GLU:HG2	1:A:500:ILE:N	2.20	0.56
1:C:52:MET:HE2	1:C:61:GLY:O	2.06	0.56
2:D:200:MET:HE3	2:D:206:ILE:HD11	1.87	0.56
3:G:209:LEU:O	3:G:213:ILE:HG22	2.05	0.56
2:E:339:ILE:HD12	2:E:349:ASP:HA	1.86	0.56
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.87	0.56
1:C:211:SER:HB3	2:F:126:MET:CE	2.28	0.56
3:G:57:ILE:HG22	3:G:184:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:65:VAL:O	4:H:72:THR:HG23	2.05	0.56
1:B:99:VAL:HG22	1:B:253:MET:HA	1.88	0.56
1:C:246:ALA:HB3	1:C:247:PRO:HD3	1.88	0.56
3:G:137:THR:HG21	5:I:39:GLY:N	2.19	0.56
1:A:62:MET:HE2	1:A:64:LEU:HD21	1.87	0.56
1:B:295:PRO:O	1:B:298:VAL:HG22	2.06	0.56
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.86	0.56
1:B:190:ASN:HA	1:B:198:LYS:HG2	1.87	0.56
2:D:188:GLU:H	2:D:221:GLN:NE2	2.04	0.56
2:F:63:MET:HE1	2:F:228:ALA:HA	1.87	0.56
1:A:49:ALA:O	1:A:50:GLU:HB2	2.07	0.55
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.71	0.55
1:B:171:ARG:NH1	1:B:171:ARG:HB2	2.21	0.55
1:C:49:ALA:O	1:C:50:GLU:HB2	2.05	0.55
2:F:433:PRO:HD2	2:F:436:GLU:HG3	1.88	0.55
3:G:160:ILE:CG2	3:G:176:LYS:HB2	2.36	0.55
2:E:223:ASN:HD22	2:E:223:ASN:H	1.55	0.55
2:F:470:ALA:HA	2:F:473:LEU:HD12	1.87	0.55
3:G:181:LEU:HG	3:G:183:THR:HB	1.89	0.55
1:A:151:LYS:HE3	1:A:427:LEU:O	2.06	0.55
2:E:89:GLU:HG2	2:E:110:THR:CG2	2.35	0.55
3:G:207:TYR:HA	5:I:12:ILE:CD1	2.37	0.55
1:B:168:ILE:HD13	1:B:169:GLY:N	2.21	0.55
12:G:2006:HOH:O	5:I:41:THR:HG21	2.06	0.55
1:B:142:VAL:HG13	12:B:2038:HOH:O	2.06	0.55
2:F:25:PHE:HB2	2:F:29:LEU:HD12	1.88	0.55
2:F:130:GLN:HB3	2:F:357:ILE:CD1	2.37	0.55
2:F:225:PRO:HG3	12:F:2025:HOH:O	2.05	0.55
3:G:117:HIS:ND1	3:G:118:ARG:HA	2.22	0.54
3:G:117:HIS:CE1	3:G:121:SER:HB2	2.42	0.54
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.39	0.54
3:G:181:LEU:HB3	3:G:184:ILE:HG22	1.89	0.54
2:F:282:GLN:HE21	2:F:282:GLN:N	1.85	0.54
1:C:226:MET:HE1	1:C:231:VAL:HG23	1.89	0.54
1:C:488:LYS:HG2	1:C:489:ILE:N	2.23	0.54
1:A:436:MET:HE3	1:A:469:LEU:HD21	1.90	0.54
3:G:144:ILE:HD13	3:G:213:ILE:HD11	1.90	0.54
3:G:181:LEU:O	3:G:184:ILE:HG22	2.08	0.54
1:C:99:VAL:HG22	1:C:253:MET:HA	1.90	0.54
2:F:87:GLY:HA2	2:F:242:TYR:CE1	2.43	0.54
3:G:164:ARG:HD3	3:G:174:GLU:OE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ALA:C	1:A:206:ILE:HG13	2.33	0.54
1:A:496:LYS:HA	1:A:499:GLU:CD	2.32	0.54
1:C:215:GLN:HE22	2:F:128:VAL:HA	1.73	0.54
2:E:31:PRO:HD2	2:E:34:ASN:ND2	2.22	0.54
2:E:126:MET:HE1	2:E:297:THR:HG21	1.90	0.54
1:B:410:LEU:HG	1:B:411:ASP:H	1.72	0.54
1:B:416:GLN:O	1:B:419:SER:HB3	2.07	0.54
1:C:52:MET:HB3	1:C:91:THR:HG21	1.90	0.54
1:C:436:MET:HE3	1:C:469:LEU:HD21	1.90	0.54
2:F:360:PRO:HD3	2:F:368:TYR:CD1	2.43	0.54
3:G:71:VAL:HG13	3:G:108:VAL:HG22	1.88	0.54
4:H:22:SER:HB2	4:H:23:PRO:HD2	1.89	0.54
2:F:345:TYR:HA	2:F:346:PRO:C	2.33	0.54
3:G:121:SER:C	3:G:123:GLN:N	2.60	0.54
2:D:139:VAL:HB	12:D:2047:HOH:O	2.06	0.53
2:D:142:LEU:HD23	12:D:2048:HOH:O	2.08	0.53
3:G:39:LYS:HB3	3:G:40:PRO:CD	2.38	0.53
1:B:168:ILE:HD11	1:B:329:THR:HG21	1.89	0.53
1:C:441:GLN:O	1:C:445:ILE:HG12	2.08	0.53
5:I:28:THR:O	5:I:29:GLU:HB2	2.08	0.53
1:B:406:PHE:CZ	1:B:410:LEU:HD22	2.43	0.53
1:B:482:LYS:NZ	1:B:496:LYS:NZ	2.56	0.53
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.38	0.53
2:E:408:ARG:HH21	2:E:412:ARG:HH22	1.56	0.53
2:F:172:ASN:HD21	2:F:431:LEU:HD11	1.73	0.53
1:B:168:ILE:HD11	1:B:329:THR:HG23	1.91	0.53
3:G:137:THR:HG22	3:G:138:PHE:N	2.24	0.53
3:G:249:THR:HA	3:G:252:ARG:NH1	2.24	0.53
1:A:381:ARG:HD2	1:A:487:GLY:O	2.08	0.52
1:B:65:ASN:ND2	2:F:17:ILE:HG23	2.25	0.52
2:D:63:MET:CE	2:D:97:VAL:HG11	2.39	0.52
2:D:310:ILE:HD13	2:D:325:THR:HG21	1.91	0.52
4:H:16:MET:HE2	4:H:18:PHE:HB2	1.91	0.52
2:D:366:GLU:O	2:D:370:VAL:HG23	2.09	0.52
2:F:84:ILE:HD13	2:F:235:THR:HG23	1.91	0.52
4:H:127:THR:O	4:H:131:ILE:HG12	2.10	0.52
5:I:5:ARG:O	5:I:6:GLN:HB3	2.10	0.52
1:C:114:ALA:HB2	1:C:121:ILE:HD12	1.91	0.52
2:D:63:MET:CE	2:D:228:ALA:HA	2.39	0.52
2:D:200:MET:HE3	2:D:206:ILE:CD1	2.39	0.52
2:E:51:GLN:HE21	2:E:272:LEU:HD22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:63:MET:CE	2:F:97:VAL:HG11	2.40	0.52
3:G:179:PHE:C	3:G:181:LEU:N	2.66	0.52
4:H:40:THR:HG23	4:H:42:THR:H	1.75	0.52
2:D:63:MET:HE3	2:D:228:ALA:HA	1.90	0.52
2:F:292:MET:CE	2:F:296:ILE:HD11	2.40	0.52
1:C:179:ALA:O	1:C:183:ILE:HG12	2.09	0.52
3:G:117:HIS:ND1	3:G:117:HIS:C	2.67	0.52
2:E:257:ASN:ND2	2:E:259:PHE:H	2.08	0.52
1:A:362:ARG:HH22	2:D:372:ARG:HD3	1.74	0.52
1:B:64:LEU:HG	1:B:65:ASN:ND2	2.24	0.52
2:D:420:VAL:HG13	10:D:700:DCW:H8	1.92	0.52
3:G:117:HIS:ND1	3:G:118:ARG:CA	2.73	0.52
3:G:117:HIS:O	3:G:120:HIS:N	2.35	0.52
4:H:34:ARG:HG2	4:H:66:HIS:O	2.10	0.51
1:B:24:ASP:O	1:B:28:THR:HB	2.11	0.51
3:G:23:MET:SD	3:G:232:MET:HE2	2.50	0.51
1:A:336:ALA:HB3	1:A:339:PRO:HG2	1.92	0.51
1:B:469:LEU:O	1:B:473:ILE:HG12	2.10	0.51
1:C:419:SER:O	1:C:423:ARG:HG2	2.10	0.51
3:G:115:ILE:C	3:G:117:HIS:N	2.68	0.51
1:C:74:VAL:HG13	1:C:241:PRO:HB3	1.93	0.51
2:E:358:MET:HE2	2:E:368:TYR:HA	1.92	0.51
2:F:337:ARG:O	2:F:341:GLU:HG3	2.10	0.51
2:F:440:GLY:HA2	2:F:463:ILE:HG13	1.91	0.51
2:D:397:SER:O	2:D:401:LYS:HD2	2.10	0.51
2:E:80:ALA:HB1	2:E:81:PRO:CD	2.40	0.51
3:G:49:LEU:HD21	3:G:212:ILE:CD1	2.41	0.51
3:G:190:MET:HE3	3:G:190:MET:HA	1.92	0.51
1:C:185:ASN:OD1	1:C:435:PRO:HB2	2.11	0.51
2:D:97:VAL:HG13	2:D:232:VAL:HG13	1.93	0.51
2:E:94:ILE:HD11	2:E:197:TYR:CD1	2.45	0.51
2:D:63:MET:HE1	2:D:97:VAL:HG11	1.92	0.51
2:D:139:VAL:HG22	2:D:414:LEU:HD22	1.92	0.51
1:B:26:GLU:HA	1:B:45:ARG:HB2	1.93	0.51
1:C:211:SER:O	1:C:215:GLN:HG2	2.11	0.51
4:H:83:THR:HB	4:H:91:GLN:HE21	1.75	0.51
1:B:357:PHE:C	1:B:359:LYS:H	2.19	0.50
1:B:457:GLU:OE1	1:B:460:LYS:HG3	2.10	0.50
1:C:418:LEU:O	1:C:422:VAL:HG23	2.10	0.50
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	0.50
2:E:27:GLU:CD	2:E:27:GLU:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:345:TYR:HA	2:E:346:PRO:C	2.35	0.50
2:E:393:MET:C	2:E:395:GLU:H	2.19	0.50
2:E:471:ASP:O	2:E:472:LYS:C	2.54	0.50
4:H:58:LEU:HD13	4:H:77:VAL:HG11	1.92	0.50
4:H:70:GLY:O	4:H:71:THR:C	2.53	0.50
2:D:95:MET:HG3	12:D:2063:HOH:O	2.11	0.50
4:H:18:PHE:CZ	4:H:20:PHE:HB2	2.46	0.50
2:D:136:GLY:HA3	2:D:431:LEU:HD12	1.92	0.50
2:D:167:MET:HG3	10:D:700:DCW:H131	1.94	0.50
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.94	0.50
2:F:408:ARG:NE	2:F:454:GLU:OE2	2.44	0.50
1:A:338:ILE:N	1:A:339:PRO:CD	2.75	0.50
5:I:35:MET:C	5:I:37:THR:N	2.68	0.50
1:B:403:PHE:O	1:B:404:ALA:C	2.53	0.50
2:D:292:MET:HE2	2:D:293:GLN:N	2.27	0.50
1:B:156:LEU:HD22	1:B:391:LYS:HD3	1.94	0.50
1:B:399:GLU:C	1:B:400:VAL:HG23	2.36	0.50
2:E:358:MET:HE2	2:E:368:TYR:HD1	1.76	0.50
2:F:96:ASN:ND2	2:F:100:GLU:H	2.09	0.50
2:E:408:ARG:HH21	2:E:412:ARG:NH2	2.10	0.50
2:F:246:GLN:O	2:F:247:GLU:HG3	2.12	0.49
2:F:63:MET:HE3	2:F:228:ALA:HA	1.93	0.49
4:H:35:GLN:HB3	4:H:66:HIS:HD2	1.77	0.49
1:B:137:ILE:HB	1:B:138:PRO:HD3	1.94	0.49
1:B:30:ARG:HH11	1:B:32:LEU:HD23	1.76	0.49
1:B:171:ARG:HB2	1:B:171:ARG:HH11	1.76	0.49
1:A:270:ASP:HB2	1:A:326:VAL:O	2.13	0.49
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.42	0.49
1:C:36:ASP:HB3	1:C:284:LEU:HD13	1.93	0.49
4:H:138:ASN:O	4:H:141:LEU:HB2	2.12	0.49
1:B:240:ALA:HB3	1:B:241:PRO:HD3	1.93	0.49
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.94	0.49
2:D:399:GLU:O	2:D:403:THR:HG23	2.12	0.49
3:G:71:VAL:HG13	3:G:108:VAL:CG2	2.43	0.49
1:A:395:ALA:HA	1:A:398:ARG:NH1	2.27	0.49
2:F:153:GLY:HA3	2:F:329:LEU:HD13	1.95	0.49
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.46	0.49
2:E:258:ILE:HD13	2:E:258:ILE:O	2.13	0.49
2:F:292:MET:HE2	2:F:296:ILE:HD11	1.94	0.49
4:H:105:LEU:CD2	4:H:109:LYS:HE3	2.41	0.49
1:B:339:PRO:O	1:B:343:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LYS:HA	1:A:499:GLU:OE2	2.13	0.49
1:A:496:LYS:HD2	1:A:499:GLU:OE2	2.13	0.49
1:B:388:GLY:O	1:B:392:LEU:HD23	2.13	0.49
4:H:41:GLN:HG2	4:H:57:VAL:HG12	1.94	0.49
1:C:404:ALA:C	1:C:406:PHE:H	2.21	0.48
2:D:10:THR:CG2	2:D:74:LYS:HE3	2.39	0.48
3:G:203:ASN:CB	4:H:57:VAL:HG21	2.42	0.48
1:A:383:MET:HE3	1:A:386:VAL:HG23	1.95	0.48
2:E:408:ARG:O	2:E:411:GLN:HG2	2.13	0.48
1:B:240:ALA:N	1:B:241:PRO:CD	2.76	0.48
2:D:136:GLY:HA3	2:D:431:LEU:HD11	1.94	0.48
2:F:266:SER:HB2	2:F:282:GLN:HE22	1.79	0.48
3:G:136:PRO:HD3	3:G:221:THR:HG21	1.95	0.48
3:G:156:ASP:O	3:G:181:LEU:HB2	2.13	0.48
4:H:34:ARG:HH22	4:H:70:GLY:CA	2.24	0.48
1:A:195:GLU:HA	1:A:198:LYS:HG3	1.94	0.48
1:C:180:ILE:HD11	1:C:216:LEU:CD2	2.44	0.48
1:B:78:ASN:ND2	2:E:119:GLU:OE2	2.46	0.48
1:B:468:PHE:CZ	1:B:501:VAL:HG12	2.48	0.48
1:C:183:ILE:HD11	1:C:267:ILE:CD1	2.43	0.48
2:E:48:GLU:HB3	2:E:61:ILE:CD1	2.44	0.48
2:E:48:GLU:O	2:E:61:ILE:HD13	2.14	0.48
2:E:359:ASP:OD2	2:E:361:ASN:HB2	2.13	0.48
3:G:197:ASP:O	3:G:200:VAL:HG12	2.13	0.48
4:H:105:LEU:HG	4:H:145:LEU:HB3	1.94	0.48
1:B:130:GLY:HA2	9:B:701:GOL:H11	1.96	0.48
1:B:168:ILE:HD13	1:B:168:ILE:C	2.38	0.48
1:C:99:VAL:CG2	1:C:253:MET:HA	2.43	0.48
3:G:160:ILE:HG22	3:G:176:LYS:HB2	1.95	0.48
1:C:105:GLY:HA2	1:C:226:MET:O	2.12	0.48
2:D:139:VAL:HG21	12:D:2115:HOH:O	2.14	0.48
2:D:420:VAL:HG22	10:D:700:DCW:H31C	1.96	0.48
2:E:339:ILE:CD1	2:E:349:ASP:HA	2.44	0.48
2:D:167:MET:HE3	12:D:2058:HOH:O	2.12	0.48
2:D:237:LEU:HD11	2:D:295:ARG:NE	2.29	0.48
2:D:276:PRO:HG3	3:G:268:GLY:HA3	1.94	0.48
2:D:292:MET:HE3	2:D:296:ILE:CD1	2.44	0.48
2:E:89:GLU:HG3	2:E:109:LYS:O	2.14	0.48
2:E:282:GLN:HE21	2:E:282:GLN:N	1.98	0.48
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.44	0.48
3:G:39:LYS:N	3:G:40:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:367:HIS:CE1	2:E:434:LEU:HD11	2.48	0.48
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.96	0.48
2:D:9:THR:HG21	2:D:28:GLY:O	2.14	0.48
1:C:183:ILE:HD11	1:C:267:ILE:HD12	1.95	0.47
2:E:167:MET:HE3	2:E:420:VAL:CG1	2.44	0.47
2:F:360:PRO:HD3	2:F:368:TYR:CE1	2.49	0.47
3:G:179:PHE:HB3	3:G:184:ILE:HG21	1.96	0.47
2:F:391:LEU:HD13	2:F:395:GLU:HG2	1.95	0.47
2:F:400:ASP:O	2:F:404:VAL:HG23	2.14	0.47
1:B:99:VAL:HG13	1:B:256:TYR:HB2	1.95	0.47
3:G:78:CYS:O	3:G:81:ILE:HD13	2.15	0.47
3:G:89:MET:CB	3:G:116:LEU:HD22	2.38	0.47
3:G:184:ILE:C	3:G:186:SER:N	2.72	0.47
4:H:57:VAL:HG13	5:I:11:TYR:CZ	2.50	0.47
5:I:37:THR:HG22	5:I:38:SER:H	1.80	0.47
1:B:292:GLU:O	1:B:293:ALA:HB3	2.14	0.47
2:D:292:MET:HE3	2:D:296:ILE:HD11	1.96	0.47
2:E:258:ILE:HD12	2:E:289:MET:HE1	1.96	0.47
1:B:185:ASN:O	1:B:188:ARG:HG2	2.15	0.47
2:D:360:PRO:HD3	2:D:368:TYR:CD1	2.50	0.47
2:D:390:ILE:HD12	3:G:16:ILE:CD1	2.44	0.47
3:G:129:LYS:HG2	3:G:130:GLU:OE1	2.14	0.47
1:B:338:ILE:N	1:B:339:PRO:CD	2.77	0.47
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.96	0.47
1:C:338:ILE:N	1:C:339:PRO:CD	2.77	0.47
2:D:87:GLY:HA2	2:D:242:TYR:CE1	2.50	0.47
2:D:126:MET:HE1	2:D:297:THR:OG1	2.14	0.47
2:E:183:PHE:HB3	2:E:217:LEU:CD2	2.45	0.47
2:E:367:HIS:ND1	2:E:438:ILE:HD11	2.30	0.47
3:G:125:LEU:HD11	3:G:151:SER:HB2	1.96	0.47
3:G:179:PHE:O	3:G:181:LEU:N	2.48	0.47
1:B:457:GLU:O	1:B:460:LYS:N	2.42	0.47
2:F:394:ASP:HB2	12:F:2143:HOH:O	2.14	0.47
3:G:180:SER:O	3:G:181:LEU:C	2.56	0.47
2:D:139:VAL:HG23	12:D:2133:HOH:O	2.15	0.47
2:D:224:GLU:HB3	2:D:225:PRO:HD2	1.97	0.47
2:E:179:GLY:HA3	2:E:250:ASP:O	2.14	0.47
4:H:47:ILE:HD12	4:H:47:ILE:H	1.79	0.47
2:D:369:ASP:OD1	2:D:372:ARG:NH2	2.47	0.47
2:D:391:LEU:HD13	3:G:23:MET:HE1	1.96	0.47
5:I:5:ARG:C	5:I:7:ALA:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:MET:CE	2:D:217:LEU:HD21	2.45	0.46
3:G:56:ASP:C	3:G:57:ILE:HG12	2.41	0.46
3:G:207:TYR:CZ	4:H:80:GLY:HA2	2.50	0.46
1:A:34:ILE:HD12	1:A:38:ILE:O	2.16	0.46
2:D:84:ILE:HB	2:D:85:PRO:HD2	1.96	0.46
2:F:188:GLU:O	2:F:222:MET:HG2	2.15	0.46
1:B:49:ALA:O	1:B:50:GLU:HB2	2.15	0.46
1:C:201:CYS:O	1:C:229:THR:HA	2.15	0.46
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.44	0.46
2:D:200:MET:HE1	2:D:215:VAL:HG11	1.96	0.46
2:E:406:ARG:O	2:E:410:ILE:HG12	2.16	0.46
3:G:144:ILE:HG21	3:G:213:ILE:HD13	1.97	0.46
1:C:188:ARG:NH2	1:C:437:ALA:N	2.64	0.46
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.98	0.46
2:F:366:GLU:O	2:F:370:VAL:HG23	2.16	0.46
1:A:20:ASP:O	1:A:21:THR:C	2.59	0.46
1:A:497:LEU:O	1:A:501:VAL:HG12	2.15	0.46
1:C:288:PRO:HG2	2:D:270:ALA:HB1	1.98	0.46
2:D:348:VAL:O	2:D:350:PRO:HD3	2.15	0.46
1:A:32:LEU:HD21	1:A:42:HIS:HB2	1.96	0.46
1:A:299:PHE:CZ	1:A:345:ILE:HD11	2.50	0.46
2:F:443:GLN:HE21	2:F:449:TYR:HE2	1.62	0.46
1:B:380:THR:HG22	1:B:383:MET:H	1.81	0.46
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.51	0.46
3:G:178:ILE:C	3:G:180:SER:N	2.69	0.46
2:E:380:ASP:O	2:E:384:LEU:HG	2.15	0.46
4:H:99:THR:O	4:H:102:MET:HG2	2.15	0.46
1:A:213:VAL:O	1:A:216:LEU:HB3	2.16	0.46
1:A:392:LEU:HG	1:A:396:GLN:NE2	2.30	0.46
1:B:44:LEU:HB3	1:B:47:VAL:CG1	2.45	0.46
1:B:354:THR:HG23	1:B:358:TYR:CE1	2.51	0.46
1:B:404:ALA:O	1:B:405:GLN:C	2.59	0.46
1:B:409:ASP:HB3	3:G:169:ILE:HD11	1.98	0.46
2:F:16:VAL:O	2:F:17:ILE:HD13	2.16	0.46
2:F:225:PRO:HB2	12:F:2020:HOH:O	2.15	0.46
2:D:97:VAL:HG22	12:D:2064:HOH:O	2.16	0.45
2:E:163:THR:O	2:E:167:MET:HG3	2.16	0.45
2:E:358:MET:HE2	2:E:368:TYR:CD1	2.51	0.45
2:F:63:MET:HE1	2:F:97:VAL:HG11	1.98	0.45
2:F:405:SER:O	2:F:409:LYS:HG3	2.16	0.45
4:H:35:GLN:HB3	4:H:66:HIS:CD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.98	0.45
3:G:206:GLU:O	5:I:12:ILE:HD11	2.17	0.45
1:B:87:ILE:HD12	1:B:87:ILE:H	1.82	0.45
2:D:279:VAL:HG12	2:D:279:VAL:O	2.16	0.45
2:E:181:SER:HB2	2:E:215:VAL:CG1	2.33	0.45
1:A:481:GLY:HA2	1:A:484:ARG:NH1	2.31	0.45
3:G:259:THR:O	3:G:263:ILE:HG12	2.17	0.45
1:B:410:LEU:HB3	1:B:415:GLN:CG	2.46	0.45
4:H:112:LEU:HD21	4:H:135:ILE:HG23	1.99	0.45
1:B:289:PRO:CG	3:G:263:ILE:HD12	2.46	0.45
3:G:51:LEU:HD13	4:H:55:LEU:HD21	1.97	0.45
1:A:114:ALA:HB2	1:A:121:ILE:CD1	2.47	0.45
3:G:228:ARG:O	3:G:232:MET:HG2	2.17	0.45
1:B:47:VAL:CG1	1:B:90:ARG:HG2	2.41	0.45
1:B:407:GLY:C	1:B:409:ASP:H	2.25	0.45
1:C:30:ARG:HA	1:C:86:ASP:O	2.15	0.45
1:C:404:ALA:C	1:C:406:PHE:N	2.74	0.45
2:E:135:THR:OG1	2:E:137:ILE:HB	2.17	0.45
2:E:400:ASP:O	2:E:404:VAL:HG23	2.17	0.45
1:B:295:PRO:HB2	1:B:297:ASP:OD1	2.16	0.45
2:F:96:ASN:HD21	2:F:100:GLU:H	1.64	0.45
1:A:362:ARG:HH22	2:D:372:ARG:CG	2.31	0.44
2:E:228:ALA:O	2:E:232:VAL:HG22	2.16	0.44
3:G:13:ILE:HD13	3:G:242:MET:SD	2.57	0.44
3:G:105:ILE:HG22	3:G:106:ILE:N	2.32	0.44
1:A:34:ILE:HD13	1:A:39:ALA:HB2	1.99	0.44
1:B:286:ARG:NE	12:B:2079:HOH:O	2.48	0.44
1:B:333:ASP:OD2	3:G:252:ARG:HD3	2.17	0.44
1:B:353:GLU:CD	1:B:366:ASN:HD22	2.26	0.44
2:F:223:ASN:H	2:F:223:ASN:ND2	2.10	0.44
3:G:117:HIS:CE1	3:G:118:ARG:NE	2.86	0.44
4:H:55:LEU:O	4:H:56:GLN:HG3	2.17	0.44
1:C:411:ASP:OD2	1:C:413:ALA:HB3	2.18	0.44
2:D:145:PRO:HD2	2:D:358:MET:HG2	1.98	0.44
2:E:61:ILE:HD13	2:E:61:ILE:H	1.83	0.44
2:E:422:GLU:HG2	2:E:427:HIS:O	2.17	0.44
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.52	0.44
2:E:397:SER:O	2:E:401:LYS:HG3	2.18	0.44
3:G:84:SER:HB3	3:G:173:THR:OG1	2.17	0.44
4:H:22:SER:HG	4:H:25:GLN:H	1.65	0.44
1:A:183:ILE:HD11	1:A:267:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:SER:CB	2:D:126:MET:HE2	2.32	0.44
1:A:291:ARG:HA	3:G:262:LEU:HD22	1.99	0.44
1:A:338:ILE:N	1:A:339:PRO:HD2	2.33	0.44
2:E:223:ASN:HD22	2:E:223:ASN:N	2.15	0.44
2:E:381:TYR:CE1	2:E:404:VAL:HG13	2.52	0.44
2:F:432:VAL:HA	2:F:433:PRO:HD3	1.83	0.44
1:A:165:GLU:O	1:A:325:PRO:HD2	2.17	0.44
1:A:383:MET:CE	1:A:386:VAL:HG23	2.47	0.44
1:B:297:ASP:HB3	2:F:267:GLU:HG2	1.99	0.44
1:B:359:LYS:HD2	1:B:361:ILE:CD1	2.48	0.44
1:C:23:VAL:HG12	1:C:23:VAL:O	2.18	0.44
2:E:183:PHE:HB3	2:E:217:LEU:HD23	2.00	0.44
3:G:128:PHE:HB3	5:I:42:ILE:CD1	2.48	0.44
4:H:33:VAL:HG11	4:H:65:VAL:HG13	1.99	0.44
1:C:33:SER:HB2	2:F:52:HIS:O	2.17	0.44
2:D:97:VAL:HG13	2:D:232:VAL:CG1	2.47	0.44
3:G:113:ARG:O	3:G:117:HIS:HB2	2.18	0.44
1:A:345:ILE:HD13	2:E:222:MET:SD	2.58	0.44
1:B:209:LYS:HD2	2:E:328:HIS:HA	2.00	0.44
2:D:142:LEU:HB3	12:D:2048:HOH:O	2.17	0.44
2:E:96:ASN:C	2:E:96:ASN:HD22	2.26	0.44
3:G:117:HIS:O	3:G:118:ARG:C	2.61	0.44
1:C:362:ARG:HD3	6:C:600:ATP:C2	2.53	0.43
1:C:381:ARG:HD2	1:C:381:ARG:N	2.32	0.43
1:C:444:VAL:HG12	1:C:469:LEU:HD13	2.00	0.43
2:D:32:ILE:O	2:D:33:LEU:HB2	2.18	0.43
2:E:374:VAL:HG13	2:E:410:ILE:HG21	1.99	0.43
1:A:422:VAL:O	1:A:426:GLU:HG2	2.18	0.43
1:B:410:LEU:HG	1:B:414:THR:OG1	2.18	0.43
2:E:257:ASN:HD22	2:E:260:ARG:H	1.65	0.43
1:A:20:ASP:O	1:A:22:SER:N	2.51	0.43
1:A:240:ALA:N	1:A:241:PRO:CD	2.81	0.43
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.48	0.43
2:D:237:LEU:HD11	2:D:295:ARG:CZ	2.48	0.43
1:B:158:PRO:O	1:B:375:GLY:HA3	2.19	0.43
1:C:62:MET:HG2	1:C:64:LEU:HD13	2.01	0.43
2:E:358:MET:CE	2:E:368:TYR:HA	2.49	0.43
2:E:415:SER:HB2	2:E:459:MET:H	1.84	0.43
2:F:223:ASN:HD22	2:F:223:ASN:N	2.07	0.43
3:G:6:ILE:HG21	3:G:250:PHE:HB2	2.00	0.43
1:A:440:GLU:O	1:A:444:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:VAL:HG22	2:D:414:LEU:HB3	2.00	0.43
2:E:419:GLN:N	2:E:429:GLY:HA3	2.33	0.43
2:F:245:ASP:O	2:F:247:GLU:N	2.50	0.43
1:B:406:PHE:CZ	1:B:410:LEU:HD13	2.53	0.43
2:D:89:GLU:HB2	2:D:110:THR:HG23	2.01	0.43
2:F:348:VAL:O	2:F:350:PRO:HD3	2.18	0.43
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.99	0.43
1:B:148:THR:HA	1:B:182:THR:HG23	2.01	0.43
1:B:508:PHE:CE2	1:B:510:ALA:HA	2.53	0.43
2:D:200:MET:HE2	2:D:217:LEU:HD21	2.00	0.43
2:E:170:ILE:CD1	2:E:215:VAL:HG11	2.46	0.43
4:H:41:GLN:CG	4:H:57:VAL:HG12	2.48	0.43
1:A:43:GLY:O	1:A:44:LEU:C	2.61	0.43
1:A:487:GLY:O	1:A:488:LYS:HB3	2.19	0.43
1:C:406:PHE:C	1:C:408:SER:H	2.26	0.43
1:C:410:LEU:O	1:C:415:GLN:NE2	2.51	0.43
2:D:188:GLU:O	2:D:221:GLN:HB3	2.18	0.43
2:F:245:ASP:C	2:F:247:GLU:N	2.77	0.43
3:G:179:PHE:C	3:G:181:LEU:H	2.27	0.43
4:H:79:SER:O	4:H:94:ALA:HA	2.18	0.43
5:I:41:THR:O	5:I:42:ILE:C	2.62	0.43
1:A:446:TYR:O	1:A:449:VAL:HG12	2.19	0.43
1:C:151:LYS:HA	1:C:441:GLN:OE1	2.17	0.43
2:F:51:GLN:HG2	2:F:59:ARG:HB3	2.00	0.43
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.01	0.43
3:G:86:ALA:O	3:G:116:LEU:HD13	2.18	0.43
4:H:35:GLN:HG2	4:H:36:VAL:N	2.34	0.43
1:B:482:LYS:NZ	1:B:496:LYS:HZ2	2.16	0.43
2:F:237:LEU:C	2:F:237:LEU:HD12	2.44	0.43
3:G:239:ALA:O	3:G:243:ILE:HG12	2.18	0.43
4:H:20:PHE:CD1	4:H:92:LEU:HD23	2.54	0.43
4:H:131:ILE:HG23	4:H:134:ARG:HH21	1.84	0.43
1:A:157:VAL:N	1:A:158:PRO:CD	2.82	0.42
1:A:423:ARG:NH2	1:A:458:PRO:HD3	2.33	0.42
1:B:269:ASP:HA	1:B:270:ASP:HA	1.74	0.42
1:B:286:ARG:HG2	2:E:275:ILE:CD1	2.49	0.42
1:C:240:ALA:N	1:C:241:PRO:CD	2.82	0.42
2:E:48:GLU:HB3	2:E:61:ILE:HD11	1.99	0.42
2:E:221:GLN:N	2:E:224:GLU:OE2	2.48	0.42
2:E:358:MET:HE3	2:E:358:MET:HA	2.01	0.42
3:G:192:ILE:HG22	4:H:53:PRO:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:O	1:A:50:GLU:CB	2.66	0.42
1:B:156:LEU:HD13	1:B:367:VAL:HG11	2.00	0.42
1:C:189:PHE:HB3	1:C:197:LYS:HB3	2.01	0.42
2:E:335:LEU:HA	2:E:347:ALA:O	2.19	0.42
2:E:387:ILE:O	2:E:391:LEU:HB3	2.18	0.42
3:G:180:SER:O	3:G:182:ASP:N	2.52	0.42
1:A:183:ILE:HD12	1:A:201:CYS:SG	2.58	0.42
1:B:157:VAL:N	1:B:158:PRO:CD	2.81	0.42
2:D:404:VAL:O	2:D:408:ARG:HG3	2.19	0.42
2:E:154:LEU:HD21	2:E:162:LYS:HG3	2.01	0.42
2:F:228:ALA:O	2:F:232:VAL:HG22	2.19	0.42
4:H:39:PRO:HG3	4:H:62:LEU:N	2.34	0.42
2:F:321:ALA:CB	2:F:322:PRO:CD	2.96	0.42
3:G:87:LYS:HA	3:G:90:LYS:HE2	2.02	0.42
1:A:102:GLU:HG2	1:A:122:GLY:O	2.19	0.42
1:B:413:ALA:O	1:B:417:LEU:HG	2.20	0.42
2:D:186:VAL:HG13	2:D:232:VAL:HG23	2.00	0.42
4:H:48:LEU:C	4:H:50:ALA:N	2.77	0.42
1:B:303:SER:HA	1:B:345:ILE:HD12	2.01	0.42
2:F:188:GLU:H	2:F:221:GLN:NE2	2.18	0.42
1:A:99:VAL:CG2	1:A:253:MET:HA	2.49	0.42
1:B:97:VAL:HB	1:B:98:PRO:CD	2.46	0.42
1:B:171:ARG:HG2	12:B:2107:HOH:O	2.19	0.42
1:C:204:VAL:HG12	1:C:206:ILE:CD1	2.50	0.42
2:F:32:ILE:CD1	2:F:51:GLN:HA	2.50	0.42
2:F:422:GLU:HG2	2:F:427:HIS:O	2.19	0.42
1:A:338:ILE:HB	1:A:339:PRO:HD3	2.02	0.42
1:A:362:ARG:HH22	2:D:372:ARG:CD	2.33	0.42
2:D:155:PHE:O	2:D:335:LEU:HB2	2.19	0.42
2:E:321:ALA:N	2:E:322:PRO:HD2	2.35	0.42
2:F:97:VAL:HG22	12:F:2073:HOH:O	2.18	0.42
2:F:416:GLN:HA	2:F:417:PRO:HD3	1.89	0.42
2:F:444:ILE:HD12	2:F:449:TYR:HD2	1.85	0.42
1:B:390:MET:O	1:B:394:LEU:HB2	2.19	0.42
1:C:406:PHE:CE1	2:D:389:ALA:HA	2.54	0.42
2:D:408:ARG:HH11	2:D:454:GLU:CD	2.28	0.42
2:E:63:MET:HE3	2:E:97:VAL:HG21	2.01	0.42
3:G:106:ILE:HG12	3:G:126:VAL:HG23	2.02	0.42
1:A:97:VAL:HB	1:A:98:PRO:HD2	2.02	0.42
1:A:269:ASP:HA	1:A:270:ASP:HA	1.77	0.42
1:B:94:ILE:O	1:B:95:VAL:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ARG:NH1	12:C:2053:HOH:O	2.53	0.42
2:D:242:TYR:CD2	2:D:246:GLN:HG3	2.55	0.42
2:F:464:GLU:CD	2:F:464:GLU:H	2.28	0.42
3:G:2:THR:C	3:G:4:LYS:N	2.75	0.42
5:I:5:ARG:O	5:I:6:GLN:CB	2.68	0.42
1:A:48:GLN:HG2	2:E:70:VAL:HG22	2.02	0.41
1:A:183:ILE:HD12	1:A:201:CYS:CB	2.47	0.41
1:B:45:ARG:HA	1:B:45:ARG:HD3	1.88	0.41
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.55	0.41
1:B:404:ALA:O	1:B:406:PHE:CD1	2.74	0.41
3:G:203:ASN:HB3	4:H:57:VAL:HG21	2.02	0.41
4:H:34:ARG:NH2	4:H:70:GLY:HA2	2.28	0.41
1:A:241:PRO:O	1:A:244:TYR:HB3	2.20	0.41
1:B:168:ILE:HD11	1:B:334:VAL:HG12	2.03	0.41
2:F:94:ILE:HG12	2:F:217:LEU:HD12	2.01	0.41
2:E:319:ASP:O	2:E:322:PRO:HD2	2.20	0.41
2:F:397:SER:C	2:F:399:GLU:N	2.78	0.41
3:G:203:ASN:HB2	4:H:57:VAL:HG21	2.02	0.41
1:B:390:MET:HE3	1:B:424:LEU:HD22	2.02	0.41
1:C:194:ASP:OD2	1:C:197:LYS:HG3	2.20	0.41
3:G:12:SER:O	3:G:16:ILE:HD12	2.20	0.41
1:B:406:PHE:HD1	1:B:407:GLY:N	2.18	0.41
1:C:180:ILE:HD11	1:C:216:LEU:HD21	2.01	0.41
2:F:471:ASP:O	2:F:473:LEU:N	2.54	0.41
3:G:89:MET:HE1	3:G:112:ILE:CG2	2.43	0.41
3:G:234:ASN:O	3:G:235:ALA:C	2.62	0.41
4:H:58:LEU:HG	4:H:80:GLY:C	2.46	0.41
4:H:62:LEU:CD1	4:H:144:ALA:HB2	2.34	0.41
1:A:168:ILE:HD11	1:A:329:THR:CG2	2.51	0.41
1:C:189:PHE:CD1	1:C:197:LYS:HD3	2.55	0.41
1:C:452:TYR:CD2	1:C:501:VAL:HG21	2.56	0.41
1:A:171:ARG:C	1:A:172:GLN:HG3	2.45	0.41
1:A:213:VAL:O	1:A:217:VAL:HG13	2.20	0.41
1:C:400:VAL:HG11	1:C:417:LEU:HD23	2.03	0.41
2:E:63:MET:CE	2:E:228:ALA:HA	2.51	0.41
2:E:258:ILE:CD1	2:E:289:MET:HE1	2.50	0.41
2:F:384:LEU:O	2:F:386:ASP:N	2.54	0.41
3:G:120:HIS:HB3	3:G:123:GLN:HB2	2.03	0.41
5:I:35:MET:O	5:I:37:THR:N	2.52	0.41
1:A:279:ARG:HG3	12:A:2097:HOH:O	2.20	0.41
1:B:158:PRO:HG2	1:B:376:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ILE:O	1:B:477:GLN:HG2	2.21	0.41
1:C:362:ARG:NH1	12:C:2122:HOH:O	2.54	0.41
2:D:417:PRO:HA	2:D:459:MET:HE1	2.02	0.41
2:E:95:MET:HG3	2:E:99:GLY:HA2	2.01	0.41
2:F:248:GLY:C	2:F:249:GLN:HG3	2.46	0.41
2:F:398:GLU:HA	2:F:401:LYS:HD2	2.02	0.41
4:H:54:THR:O	4:H:55:LEU:HD23	2.20	0.41
12:A:2128:HOH:O	2:D:354:THR:HG22	2.20	0.41
1:B:168:ILE:CD1	1:B:334:VAL:HG12	2.50	0.41
1:C:304:ARG:HH11	1:C:304:ARG:HD3	1.71	0.41
2:D:274:ARG:O	3:G:272:LEU:HD11	2.21	0.41
2:E:454:GLU:C	2:E:456:ALA:H	2.29	0.41
2:F:357:ILE:CD1	2:F:362:ILE:HD13	2.51	0.41
1:A:307:GLU:HG3	2:E:223:ASN:HB3	2.03	0.40
1:B:410:LEU:HG	1:B:411:ASP:N	2.36	0.40
1:B:457:GLU:O	1:B:458:PRO:C	2.64	0.40
1:C:114:ALA:HB2	1:C:121:ILE:CD1	2.52	0.40
1:C:144:GLU:HA	1:C:145:PRO:HD3	1.92	0.40
1:C:263:HIS:HD2	1:C:320:SER:OG	2.04	0.40
1:C:452:TYR:OH	1:C:498:LYS:HG3	2.21	0.40
2:D:382:LYS:HA	2:D:385:GLN:HE21	1.86	0.40
2:E:32:ILE:O	2:E:33:LEU:HB2	2.21	0.40
3:G:73:SER:O	3:G:111:LYS:HB2	2.21	0.40
4:H:62:LEU:HD23	4:H:75:TYR:O	2.22	0.40
1:A:295:PRO:HD3	12:A:2097:HOH:O	2.21	0.40
1:B:185:ASN:OD1	1:B:435:PRO:HB2	2.21	0.40
1:B:268:TYR:O	1:B:270:ASP:HA	2.20	0.40
2:D:246:GLN:O	2:D:247:GLU:HG3	2.21	0.40
2:E:170:ILE:O	2:E:171:ASN:C	2.65	0.40
2:E:454:GLU:C	2:E:456:ALA:N	2.80	0.40
2:F:208:LEU:C	2:F:209:LYS:HE2	2.46	0.40
3:G:2:THR:HG22	3:G:4:LYS:H	1.86	0.40
3:G:180:SER:O	3:G:205:GLN:NE2	2.50	0.40
1:A:138:PRO:HB3	1:A:316:PHE:CE1	2.55	0.40
1:A:398:ARG:NH2	12:A:2137:HOH:O	2.45	0.40
1:B:509:GLU:O	1:B:510:ALA:C	2.65	0.40
1:C:237:SER:HB3	2:F:294:GLU:HG3	2.03	0.40
1:C:269:ASP:HA	1:C:270:ASP:HA	1.74	0.40
2:D:428:LEU:HD12	2:D:428:LEU:HA	1.97	0.40
3:G:51:LEU:HD23	3:G:52:TYR:CZ	2.57	0.40
3:G:184:ILE:O	3:G:184:ILE:HD13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:78:SER:HB3	5:I:22:VAL:HG21	2.03	0.40
1:A:20:ASP:C	1:A:22:SER:N	2.77	0.40
1:C:48:GLN:HB2	1:C:51:GLU:HB2	2.02	0.40
2:F:443:GLN:NE2	2:F:449:TYR:OH	2.54	0.40
4:H:40:THR:HG23	4:H:42:THR:N	2.36	0.40
1:A:168:ILE:HD11	1:A:329:THR:HG21	2.03	0.40
1:A:183:ILE:HD11	1:A:267:ILE:CD1	2.51	0.40
2:E:63:MET:HE1	2:E:228:ALA:HA	2.03	0.40
4:H:95:GLU:O	4:H:96:GLU:HG2	2.22	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	490/510 (96%)	468 (96%)	19 (4%)	3 (1%)	21	32
1	B	490/510 (96%)	451 (92%)	31 (6%)	8 (2%)	7	11
1	C	490/510 (96%)	468 (96%)	21 (4%)	1 (0%)	43	58
2	D	465/482 (96%)	437 (94%)	27 (6%)	1 (0%)	43	58
2	E	464/482 (96%)	434 (94%)	23 (5%)	7 (2%)	8	12
2	F	464/482 (96%)	433 (93%)	27 (6%)	4 (1%)	14	22
3	G	257/272 (94%)	223 (87%)	26 (10%)	8 (3%)	3	3
4	H	129/146 (88%)	118 (92%)	8 (6%)	3 (2%)	5	6
5	I	45/50 (90%)	36 (80%)	4 (9%)	5 (11%)	0	0
All	All	3294/3444 (96%)	3068 (93%)	186 (6%)	40 (1%)	10	16

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	B	404	ALA
1	B	405	GLN
1	B	406	PHE
1	B	411	ASP
2	E	391	LEU
2	E	472	LYS
4	H	71	THR
5	I	29	GLU
1	A	488	LYS
1	C	407	GLY
2	F	28	GLY
2	F	246	GLN
2	F	385	GLN
3	G	51	LEU
3	G	56	ASP
1	A	21	THR
1	B	408	SER
1	B	452	TYR
2	D	448	GLU
2	E	389	ALA
3	G	72	SER
3	G	180	SER
5	I	36	LYS
1	B	31	VAL
2	E	109	LYS
3	G	122	ASP
4	H	49	ALA
5	I	40	SER
1	B	400	VAL
2	E	394	ASP
2	E	455	GLN
3	G	116	LEU
3	G	179	PHE
3	G	185	SER
4	H	79	SER
5	I	28	THR
5	I	42	ILE
2	E	279	VAL
2	F	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	397/412 (96%)	375 (94%)	22 (6%)	19	34
1	B	397/412 (96%)	372 (94%)	25 (6%)	16	29
1	C	397/412 (96%)	370 (93%)	27 (7%)	14	25
2	D	377/386 (98%)	366 (97%)	11 (3%)	37	60
2	E	376/386 (97%)	355 (94%)	21 (6%)	19	33
2	F	376/386 (97%)	363 (96%)	13 (4%)	32	53
3	G	225/230 (98%)	208 (92%)	17 (8%)	12	21
4	H	104/109 (95%)	99 (95%)	5 (5%)	23	40
5	I	38/41 (93%)	34 (90%)	4 (10%)	6	10
All	All	2687/2774 (97%)	2542 (95%)	145 (5%)	20	35

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	50	GLU
1	A	52	MET
1	A	59	LEU
1	A	79	ASP
1	A	80	LYS
1	A	99	VAL
1	A	141	SER
1	A	143	ARG
1	A	157	VAL
1	A	168	ILE
1	A	367	VAL
1	A	371	VAL
1	A	434	SER
1	A	438	ILE
1	A	439	GLU
1	A	444	VAL
1	A	449	VAL

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Mol	Chain	Res	Type
1	A	462	THR
1	A	469	LEU
1	A	479	LEU
1	A	493	SER
1	B	21	THR
1	B	28	THR
1	B	34	ILE
1	B	99	VAL
1	B	102	GLU
1	B	142	VAL
1	B	146	MET
1	B	157	VAL
1	B	167	ILE
1	B	168	ILE
1	B	171	ARG
1	B	216	LEU
1	B	276	VAL
1	B	298	VAL
1	B	344	SER
1	B	361	ILE
1	B	371	VAL
1	B	380	THR
1	B	384	LYS
1	B	400	VAL
1	B	406	PHE
1	B	442	VAL
1	B	449	VAL
1	B	505	LEU
1	B	509	GLU
1	C	34	ILE
1	C	52	MET
1	C	56	SER
1	C	57	SER
1	C	64	LEU
1	C	74	VAL
1	C	91	THR
1	C	99	VAL
1	C	140	ILE
1	C	202	ILE
1	C	206	ILE
1	C	216	LEU
1	C	217	VAL

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Mol	Chain	Res	Type
1	C	298	VAL
1	C	334	VAL
1	C	349	GLN
1	C	381	ARG
1	C	408	SER
1	C	414	THR
1	C	434	SER
1	C	444	VAL
1	C	449	VAL
1	C	461	ILE
1	C	470	SER
1	C	479	LEU
1	C	485	THR
1	C	505	LEU
2	D	9	THR
2	D	61	ILE
2	D	97	VAL
2	D	132	ILE
2	D	205	VAL
2	D	258	ILE
2	D	282	GLN
2	D	335	LEU
2	D	384	LEU
2	D	393	MET
2	D	420	VAL
2	E	9	THR
2	E	27	GLU
2	E	61	ILE
2	E	67	GLU
2	E	84	ILE
2	E	89	GLU
2	E	96	ASN
2	E	97	VAL
2	E	139	VAL
2	E	151	LYS
2	E	223	ASN
2	E	232	VAL
2	E	251	VAL
2	E	252	LEU
2	E	257	ASN
2	E	258	ILE
2	E	282	GLN

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Mol	Chain	Res	Type
2	E	297	THR
2	E	391	LEU
2	E	420	VAL
2	E	431	LEU
2	F	51	GLN
2	F	76	LEU
2	F	96	ASN
2	F	97	VAL
2	F	139	VAL
2	F	223	ASN
2	F	232	VAL
2	F	279	VAL
2	F	282	GLN
2	F	420	VAL
2	F	436	GLU
2	F	444	ILE
2	F	463	ILE
3	G	20	THR
3	G	35	GLU
3	G	59	THR
3	G	67	LEU
3	G	108	VAL
3	G	113	ARG
3	G	118	ARG
3	G	125	LEU
3	G	126	VAL
3	G	130	GLU
3	G	180	SER
3	G	184	ILE
3	G	190	MET
3	G	205	GLN
3	G	212	ILE
3	G	213	ILE
3	G	262	LEU
4	H	54	THR
4	H	57	VAL
4	H	91	GLN
4	H	105	LEU
4	H	112	LEU
5	I	1	VAL
5	I	37	THR
5	I	41	THR

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Mol	Chain	Res	Type
5	I	42	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	260	ASN
1	A	330	GLN
1	A	379	GLN
1	A	396	GLN
1	A	405	GLN
1	A	476	HIS
1	B	48	GLN
1	B	65	ASN
1	B	186	GLN
1	B	243	GLN
1	B	330	GLN
1	B	466	ASN
1	B	475	GLN
1	B	503	ASN
1	C	65	ASN
1	C	186	GLN
1	C	215	GLN
1	C	260	ASN
1	C	263	HIS
1	C	349	GLN
1	C	405	GLN
1	C	416	GLN
2	D	130	GLN
2	D	171	ASN
2	D	194	ASN
2	D	221	GLN
2	D	282	GLN
2	D	385	GLN
2	D	455	GLN
2	E	51	GLN
2	E	194	ASN
2	E	223	ASN
2	E	257	ASN
2	E	263	GLN
2	E	282	GLN
2	E	361	ASN

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Mol	Chain	Res	Type
2	E	411	GLN
2	F	51	GLN
2	F	96	ASN
2	F	194	ASN
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	361	ASN
2	F	419	GLN
2	F	443	GLN
3	G	82	HIS
3	G	88	GLN
3	G	234	ASN
4	H	91	GLN
4	H	111	ASN
4	H	132	GLN
4	H	138	ASN
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 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\# Z > 2$
11	SO4	E	630	-	4,4,4	0.72	0	6,6,6	0.11	0
10	DCW	D	700	2	17,17,17	1.09	0	21,21,21	1.22	1 (4%)
8	ADP	F	600	7	28,29,29	0.98	2 (7%)	43,45,45	0.68	0
8	ADP	B	600	7	28,29,29	0.95	1 (3%)	43,45,45	0.67	1 (2%)
6	ATP	A	600	7	32,33,33	0.93	1 (3%)	48,52,52	0.73	1 (2%)
6	ATP	C	600	7	32,33,33	1.13	2 (6%)	48,52,52	0.75	0
9	GOL	B	701	-	5,5,5	0.27	0	5,5,5	0.41	0
8	ADP	D	600	7	28,29,29	0.98	0	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
10	DCW	D	700	2	-	3/8/24/24	0/2/2/2
8	ADP	F	600	7	-	2/16/32/32	0/3/3/3
8	ADP	B	600	7	-	2/16/32/32	0/3/3/3
6	ATP	A	600	7	-	7/22/38/38	0/3/3/3
6	ATP	C	600	7	-	4/22/38/38	0/3/3/3
9	GOL	B	701	-	-	2/4/4/4	-
8	ADP	D	600	7	-	3/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	600	ATP	PA-O3A	3.43	1.63	1.59
8	F	600	ADP	PA-O3A	2.18	1.61	1.59
8	B	600	ADP	C2-N3	-2.12	1.30	1.33
6	A	600	ATP	C2-N3	-2.10	1.30	1.33
8	F	600	ADP	C2-N3	-2.06	1.30	1.33
6	C	600	ATP	C2-N3	-2.04	1.30	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	700	DCW	C8-N2-C1	3.36	130.15	122.92
8	B	600	ADP	O2A-PA-O3A	2.19	113.20	107.27
6	A	600	ATP	O2A-PA-O3A	2.02	112.74	107.27

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	600	ATP	PB-O3B-PG-O2G
6	C	600	ATP	PB-O3B-PG-O2G
8	B	600	ADP	PA-O3A-PB-O2B
8	D	600	ADP	PA-O3A-PB-O2B
8	F	600	ADP	PA-O3A-PB-O2B
8	F	600	ADP	PA-O3A-PB-O3B
9	B	701	GOL	C1-C2-C3-O3
9	B	701	GOL	O2-C2-C3-O3
10	D	700	DCW	O1-C1-N1-C2
10	D	700	DCW	N2-C1-N1-C2
10	D	700	DCW	C3-C2-N1-C1
6	A	600	ATP	PA-O3A-PB-O1B
8	B	600	ADP	PA-O3A-PB-O1B
6	C	600	ATP	PA-O3A-PB-O1B
6	A	600	ATP	PB-O3B-PG-O1G
8	D	600	ADP	PA-O3A-PB-O1B
6	A	600	ATP	PB-O3B-PG-O3G
6	C	600	ATP	PB-O3B-PG-O3G
8	D	600	ADP	PA-O3A-PB-O3B
6	A	600	ATP	PG-O3B-PB-O1B
6	A	600	ATP	PG-O3B-PB-O2B
6	A	600	ATP	PA-O3A-PB-O2B
6	C	600	ATP	PB-O3B-PG-O1G

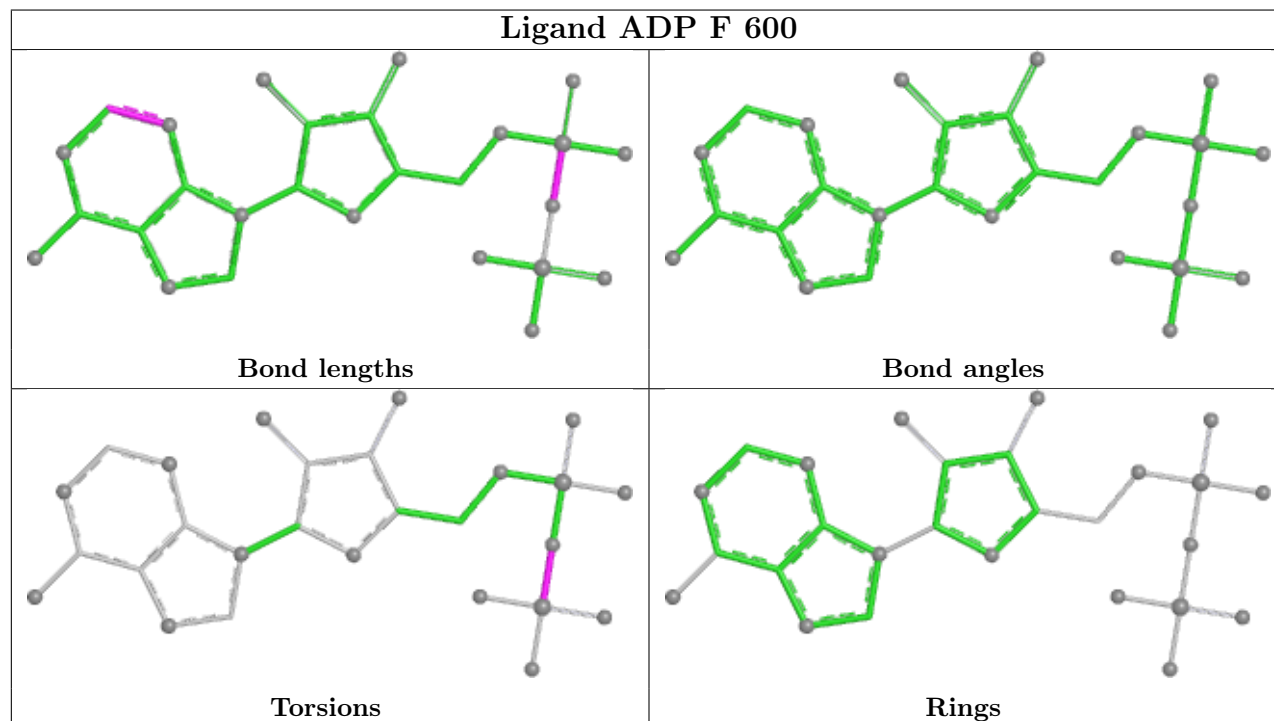
There are no ring outliers.

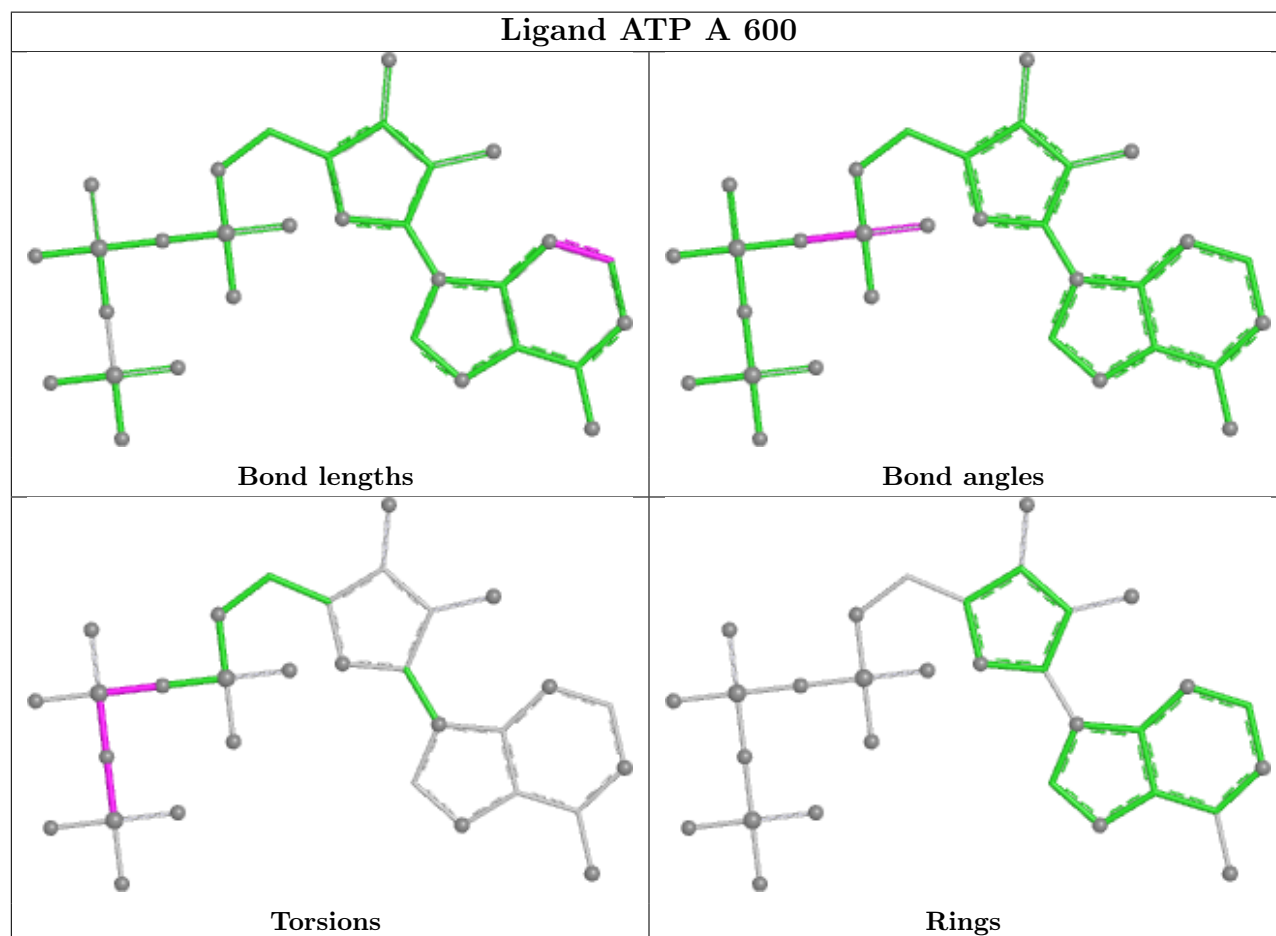
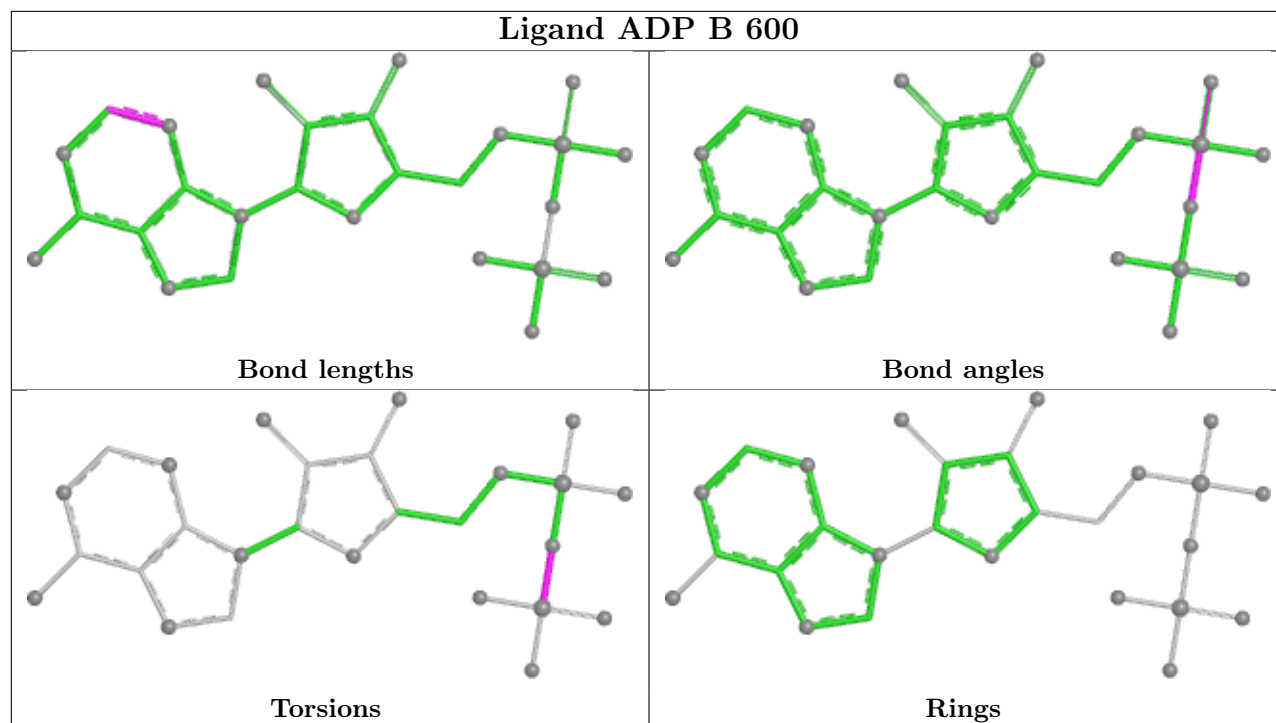
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	700	DCW	6	0
6	C	600	ATP	1	0
9	B	701	GOL	1	0

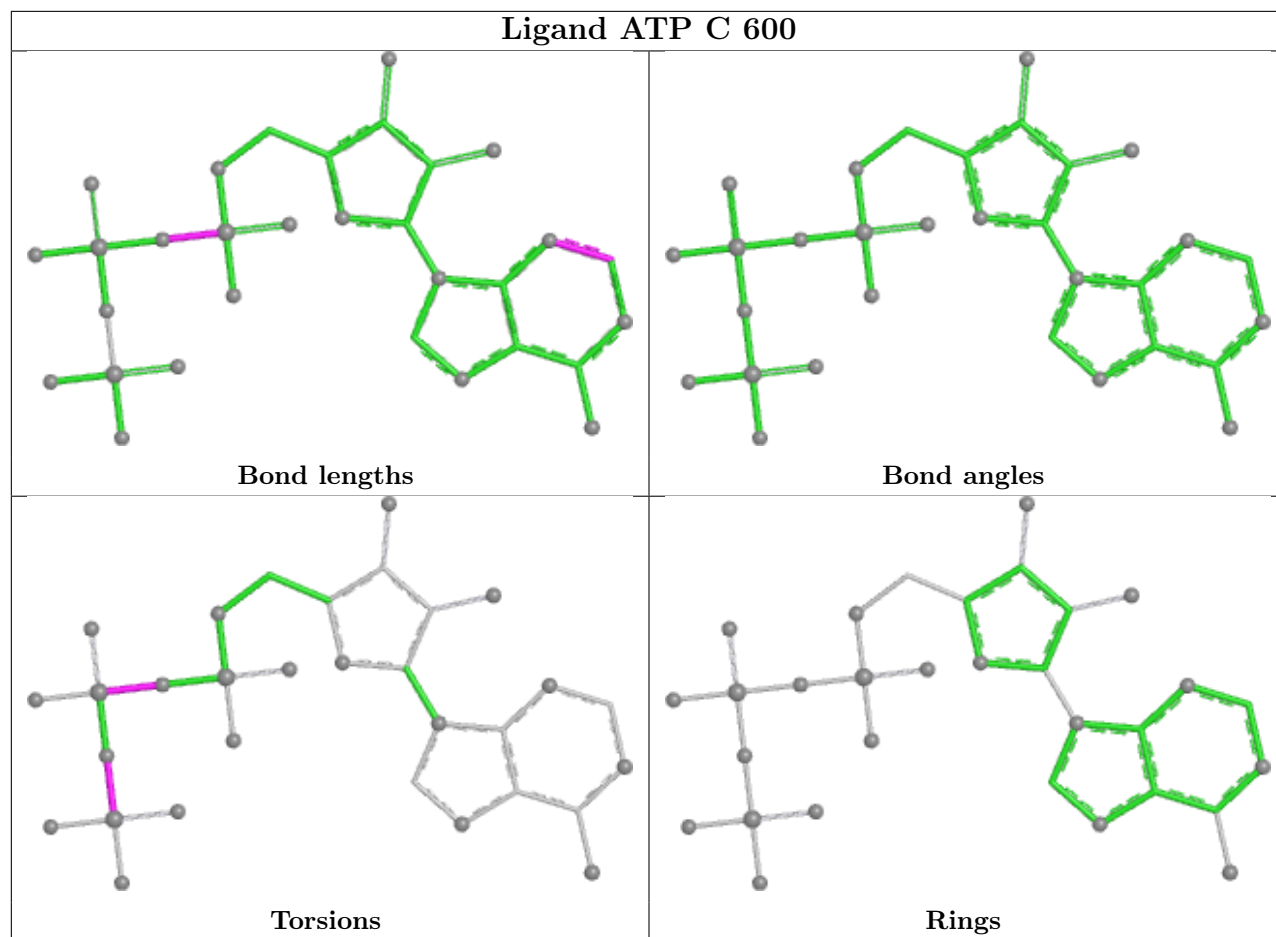
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

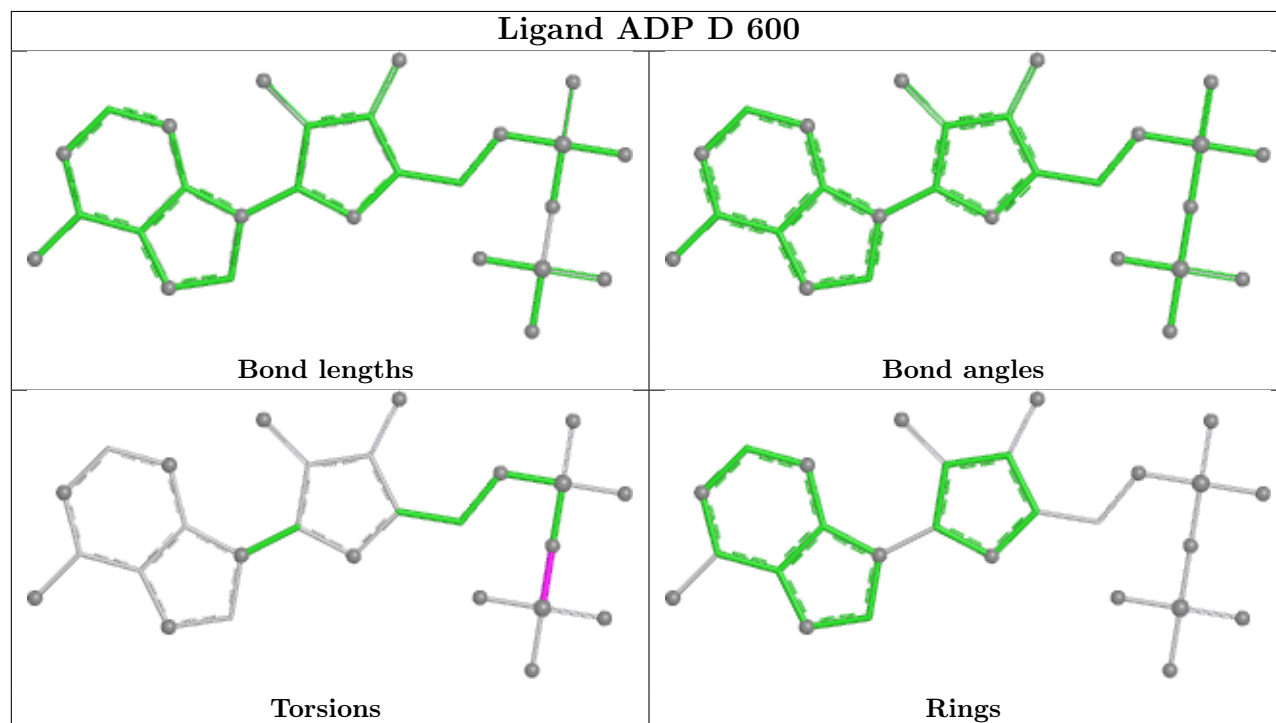




Ligand ATP C 600



Ligand ADP D 600



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	492/510 (96%)	0.03	12 (2%) 59 55	32, 46, 74, 104	0
1	B	492/510 (96%)	0.24	35 (7%) 22 18	32, 48, 95, 143	0
1	C	492/510 (96%)	-0.10	7 (1%) 73 69	30, 44, 63, 102	0
2	D	467/482 (96%)	-0.00	6 (1%) 75 71	31, 45, 69, 100	0
2	E	466/482 (96%)	0.46	33 (7%) 22 18	34, 54, 101, 132	0
2	F	466/482 (96%)	0.01	11 (2%) 59 55	32, 44, 74, 89	0
3	G	263/272 (96%)	1.17	54 (20%) 2 2	36, 68, 116, 133	0
4	H	131/146 (89%)	1.90	58 (44%) 0 0	67, 97, 131, 136	0
5	I	47/50 (94%)	1.97	23 (48%) 0 0	58, 91, 127, 129	0
All	All	3316/3444 (96%)	0.29	239 (7%) 21 18	30, 48, 102, 143	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	474	ALA	6.5
1	A	19	ALA	6.2
2	E	390	ILE	5.6
3	G	180	SER	5.5
5	I	47	VAL	5.5
3	G	199	ASP	5.4
3	G	116	LEU	5.3
1	B	21	THR	4.9
1	B	20	ASP	4.8
1	B	404	ALA	4.7
3	G	1	ALA	4.7
1	C	407	GLY	4.6
5	I	28	THR	4.6
3	G	187	ALA	4.5
4	H	47	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	414	THR	4.3
1	A	23	VAL	4.2
4	H	55	LEU	4.2
4	H	44	ALA	4.2
2	E	387	ILE	4.2
1	B	400	VAL	4.1
1	B	19	ALA	4.1
4	H	145	LEU	4.0
2	E	474	ALA	4.0
4	H	128	ARG	4.0
3	G	57	ILE	4.0
1	B	410	LEU	3.9
1	A	21	THR	3.9
1	C	408	SER	3.9
2	E	473	LEU	3.9
4	H	71	THR	3.9
3	G	123	GLN	3.8
3	G	120	HIS	3.8
2	D	248	GLY	3.8
3	G	194	ASP	3.8
2	E	397	SER	3.7
3	G	198	ALA	3.7
3	G	61	GLU	3.7
3	G	189	SER	3.7
4	H	48	LEU	3.7
2	F	248	GLY	3.6
3	G	195	ASP	3.6
1	B	358	TYR	3.6
3	G	186	SER	3.6
3	G	119	THR	3.6
1	B	193	THR	3.5
3	G	193	TYR	3.5
3	G	117	HIS	3.5
1	C	406	PHE	3.5
1	B	413	ALA	3.5
4	H	46	GLY	3.5
4	H	67	ALA	3.5
2	E	455	GLN	3.5
4	H	144	ALA	3.5
2	F	249	GLN	3.4
3	G	185	SER	3.4
1	C	409	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
3	G	51	LEU	3.4
3	G	103	VAL	3.4
4	H	112	LEU	3.4
3	G	192	ILE	3.4
2	D	249	GLN	3.3
3	G	181	LEU	3.3
1	B	406	PHE	3.3
4	H	140	ALA	3.3
3	G	184	ILE	3.3
1	A	499	GLU	3.3
3	G	59	THR	3.3
3	G	58	LYS	3.2
2	E	384	LEU	3.2
1	B	401	ALA	3.2
4	H	31	ALA	3.2
4	H	45	PHE	3.2
3	G	200	VAL	3.2
5	I	42	ILE	3.2
2	D	28	GLY	3.1
5	I	30	PHE	3.1
2	E	393	MET	3.1
3	G	182	ASP	3.1
4	H	38	VAL	3.0
1	B	416	GLN	3.0
2	E	419	GLN	3.0
4	H	103	LEU	3.0
1	B	403	PHE	3.0
5	I	40	SER	3.0
1	A	405	GLN	3.0
4	H	49	ALA	3.0
5	I	3	TYR	3.0
2	E	391	LEU	3.0
2	F	28	GLY	3.0
3	G	196	ILE	3.0
2	E	27	GLU	2.9
4	H	142	VAL	2.9
4	H	143	LYS	2.9
2	E	424	PHE	2.9
5	I	41	THR	2.9
4	H	109	LYS	2.9
5	I	43	LYS	2.9
3	G	60	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
4	H	115	ALA	2.9
1	B	405	GLN	2.9
3	G	179	PHE	2.9
1	B	457	GLU	2.9
1	B	407	GLY	2.9
5	I	31	LYS	2.8
1	A	404	ALA	2.8
3	G	118	ARG	2.8
5	I	1	VAL	2.8
5	I	22	VAL	2.8
3	G	96	LEU	2.8
4	H	62	LEU	2.8
2	E	453	PRO	2.8
2	E	389	ALA	2.8
1	A	20	ASP	2.8
1	B	23	VAL	2.8
1	B	510	ALA	2.8
2	F	42	GLU	2.8
3	G	114	SER	2.7
4	H	33	VAL	2.7
4	H	52	VAL	2.7
1	B	417	LEU	2.7
2	F	176	ALA	2.7
3	G	105	ILE	2.7
4	H	77	VAL	2.7
3	G	50	ALA	2.7
4	H	65	VAL	2.7
5	I	46	LYS	2.7
5	I	6	GLN	2.7
2	E	386	ASP	2.7
4	H	131	ILE	2.7
2	E	472	LYS	2.7
2	F	473	LEU	2.7
3	G	52	TYR	2.7
4	H	72	THR	2.7
2	E	407	ALA	2.6
2	F	9	THR	2.6
2	F	387	ILE	2.6
2	E	403	THR	2.6
2	F	385	GLN	2.6
3	G	80	ALA	2.6
4	H	54	THR	2.6

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Mol	Chain	Res	Type	RSRZ
4	H	97	ALA	2.6
1	B	418	LEU	2.6
2	E	428	LEU	2.6
2	E	392	GLY	2.6
3	G	124	PHE	2.6
2	E	402	LEU	2.6
3	G	201	LEU	2.6
4	H	138	ASN	2.6
1	A	22	SER	2.6
5	I	12	ILE	2.5
2	D	399	GLU	2.5
4	H	113	GLU	2.5
1	B	22	SER	2.5
3	G	54	LYS	2.5
3	G	94	ALA	2.5
5	I	34	ALA	2.5
3	G	2	THR	2.5
3	G	56	ASP	2.5
4	H	57	VAL	2.5
1	C	19	ALA	2.5
4	H	86	ALA	2.5
4	H	130	GLU	2.5
4	H	37	ASP	2.5
1	C	410	LEU	2.5
2	D	475	GLU	2.4
4	H	85	ASN	2.4
4	H	50	ALA	2.4
5	I	2	ALA	2.4
3	G	156	ASP	2.4
4	H	24	THR	2.4
4	H	39	PRO	2.4
2	E	342	LEU	2.4
2	E	345	TYR	2.4
4	H	64	VAL	2.4
3	G	183	THR	2.3
4	H	53	PRO	2.3
4	H	70	GLY	2.3
2	E	420	VAL	2.3
4	H	84	VAL	2.3
2	E	396	LEU	2.3
3	G	178	ILE	2.3
4	H	51	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
5	I	44	ILE	2.3
1	A	24	ASP	2.3
1	B	397	TYR	2.3
4	H	111	ASN	2.3
1	B	490	SER	2.3
1	B	402	ALA	2.3
1	B	411	ASP	2.3
2	E	456	ALA	2.2
5	I	39	GLY	2.2
1	A	482	LYS	2.2
2	D	397	SER	2.2
1	B	409	ASP	2.2
4	H	68	GLU	2.2
4	H	132	GLN	2.2
4	H	43	GLY	2.2
3	G	102	GLU	2.2
1	B	412	ALA	2.2
4	H	66	HIS	2.2
2	E	9	THR	2.2
4	H	119	LEU	2.2
4	H	17	SER	2.2
1	A	402	ALA	2.2
4	H	16	MET	2.2
3	G	167	SER	2.2
3	G	191	SER	2.2
4	H	124	ASP	2.2
2	E	460	VAL	2.1
1	B	389	THR	2.1
1	B	394	LEU	2.1
2	E	426	GLY	2.1
2	E	388	ILE	2.1
1	A	457	GLU	2.1
1	B	30	ARG	2.1
3	G	53	GLU	2.1
1	B	408	SER	2.1
2	F	175	LYS	2.1
1	B	415	GLN	2.1
1	C	193	THR	2.1
2	E	163	THR	2.1
4	H	34	ARG	2.1
5	I	29	GLU	2.1
4	H	69	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	152	GLY	2.1
3	G	197	ASP	2.1
5	I	21	ALA	2.1
5	I	37	THR	2.1
2	E	444	ILE	2.1
3	G	149	LEU	2.0
1	B	483	ILE	2.0
3	G	68	ILE	2.0
5	I	14	TYR	2.0
4	H	56	GLN	2.0
1	B	398	ARG	2.0
4	H	76	PHE	2.0
5	I	32	ALA	2.0
2	E	362	ILE	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.

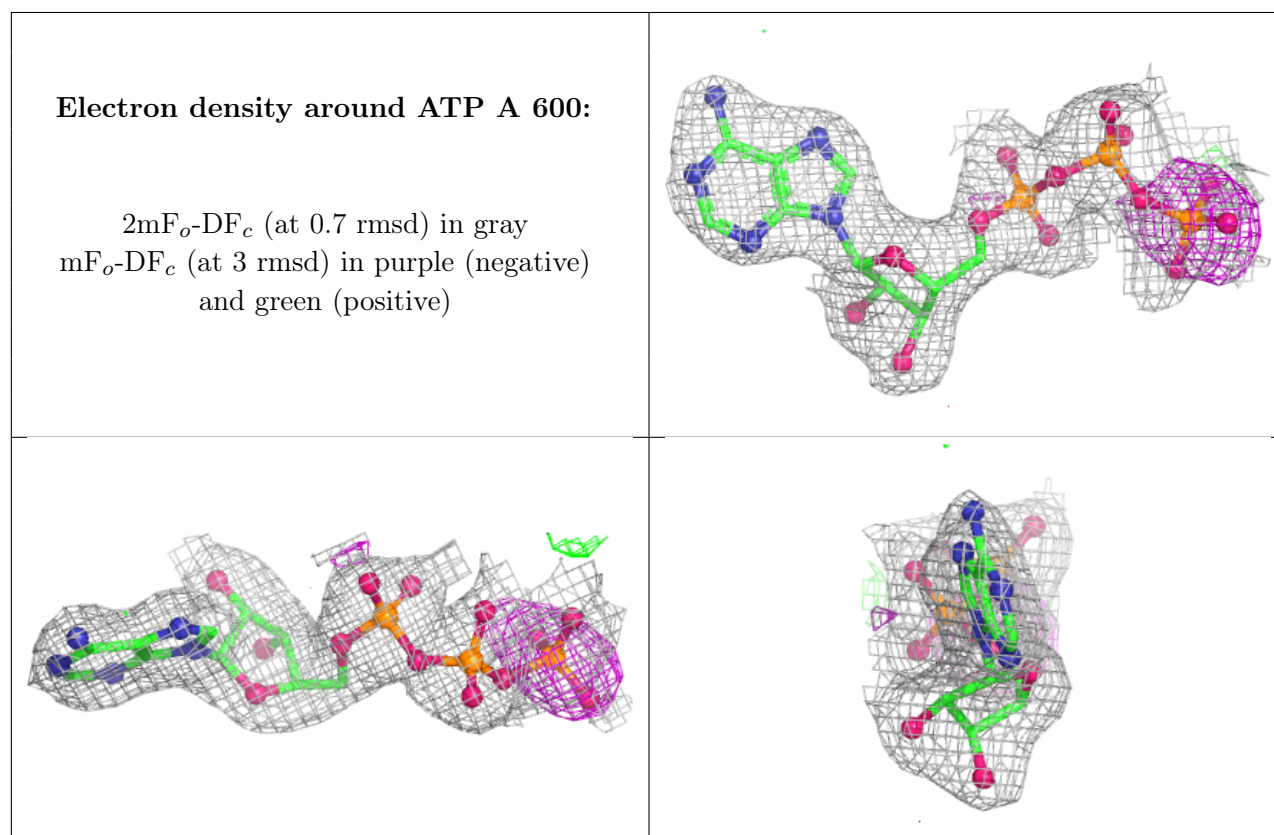
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	SO4	E	630	5/5	0.71	0.24	100,100,100,100	0
10	DCW	D	700	16/16	0.72	0.19	69,73,78,78	0
7	MG	A	601	1/1	0.87	0.09	44,44,44,44	0
7	MG	C	601	1/1	0.90	0.08	43,43,43,43	0
6	ATP	A	600	31/31	0.93	0.09	42,44,56,56	0
6	ATP	C	600	31/31	0.93	0.09	36,42,51,52	0
7	MG	D	601	1/1	0.94	0.05	35,35,35,35	0
9	GOL	B	701	6/6	0.95	0.08	39,43,44,45	0
8	ADP	B	600	27/27	0.96	0.07	44,52,56,56	0

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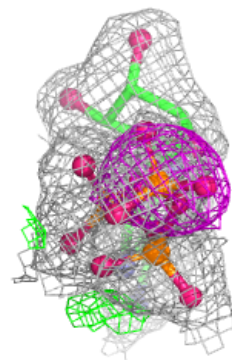
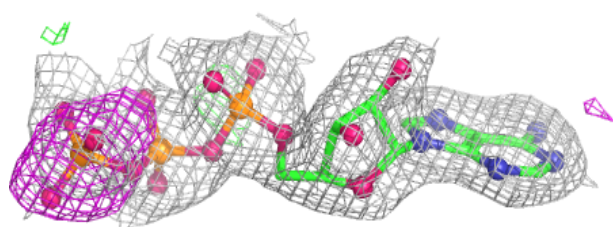
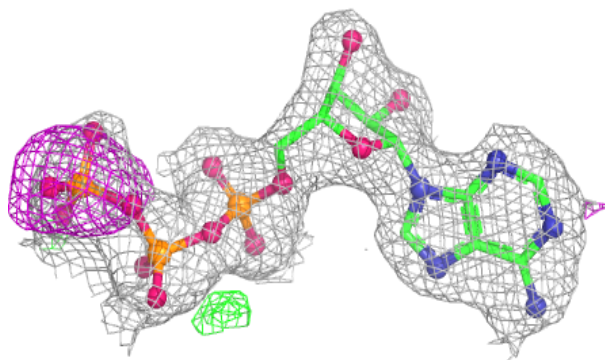
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	F	601	1/1	0.97	0.04	34,34,34,34	0
8	ADP	D	600	27/27	0.97	0.07	35,37,38,39	0
8	ADP	F	600	27/27	0.97	0.06	41,42,45,45	0
7	MG	B	601	1/1	0.98	0.03	46,46,46,46	0

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

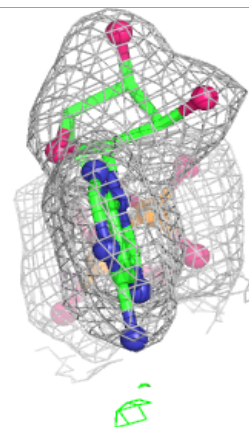
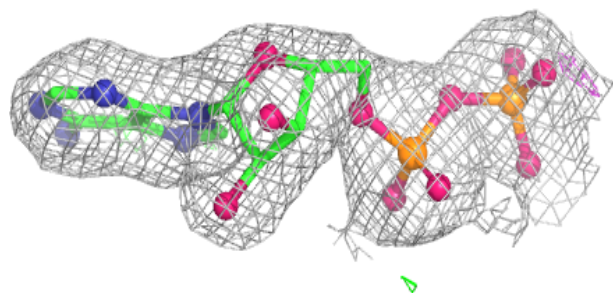
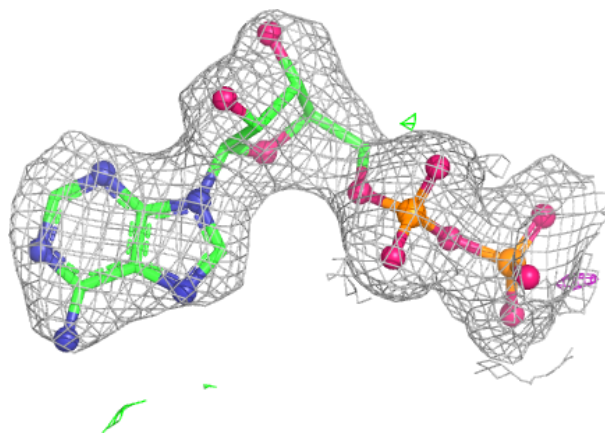


Electron density around ATP C 600:

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

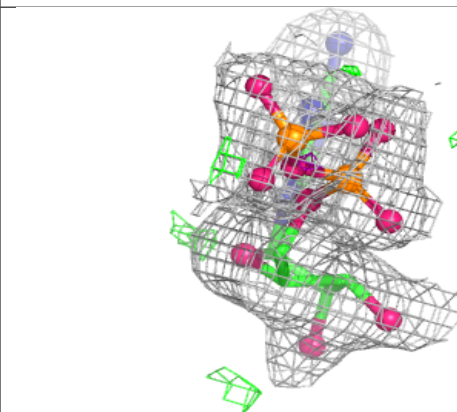
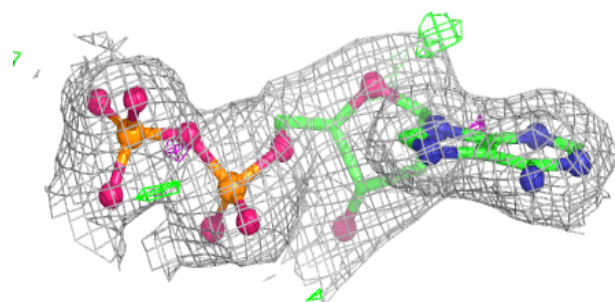
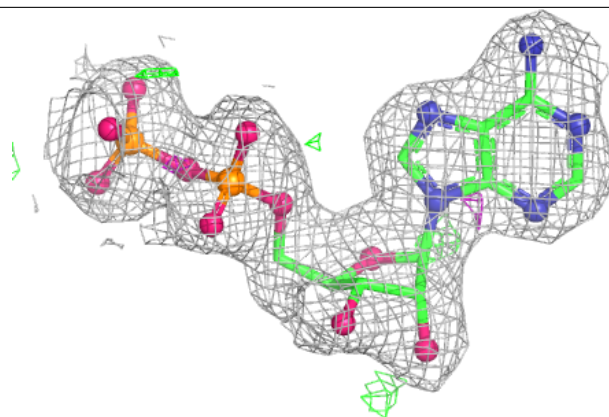
**Electron density around ADP B 600:**

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

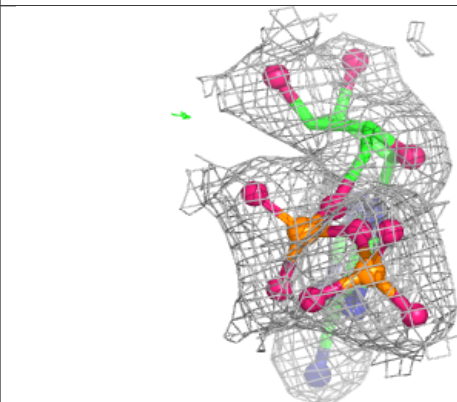
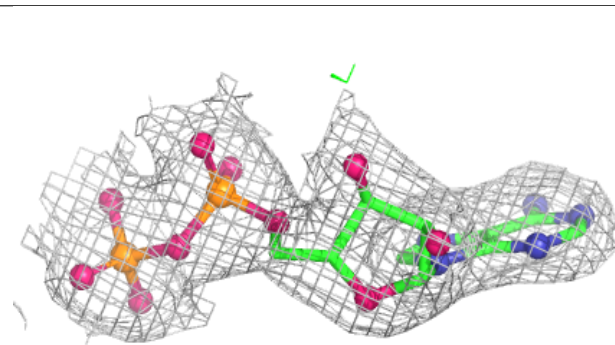
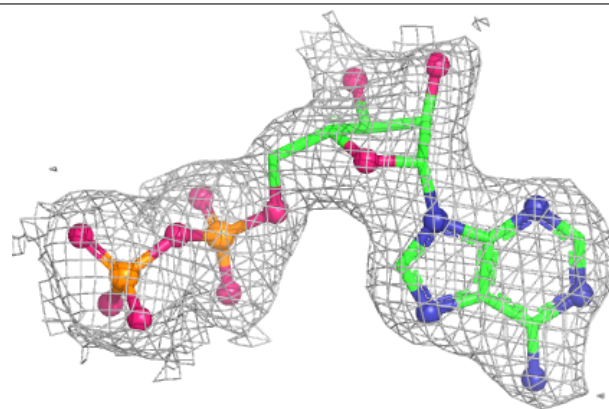


Electron density around ADP D 600:

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

**Electron density around ADP F 600:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.