



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 06:44 PM UTC

PDB ID : 1KMN / pdb_00001kmn
Title : HISTIDYL-TRNA SYNTHETASE COMPLEXED WITH HISTIDINOL AND ATP
Authors : Arnez, J.G.; Francklyn, C.S.; Moras, D.
Deposited on : 1997-05-09
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

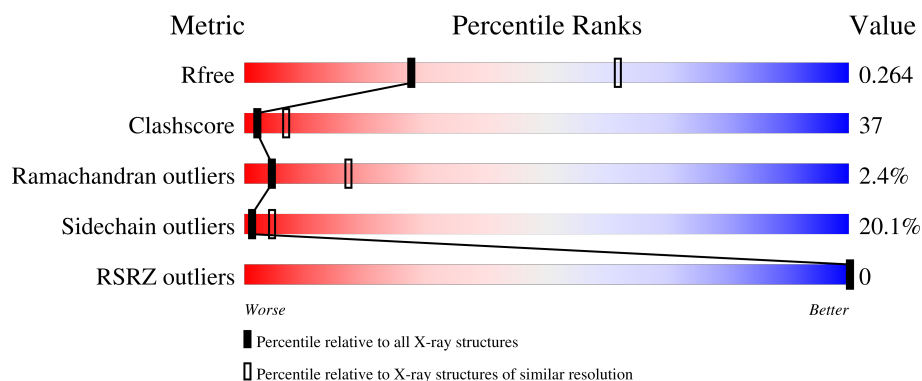
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	424	
1	B	424	
1	C	424	
1	D	424	

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
3	ATP	B	452	-	-	X	-
3	ATP	D	452	-	-	X	-

2 Entry composition [i](#)

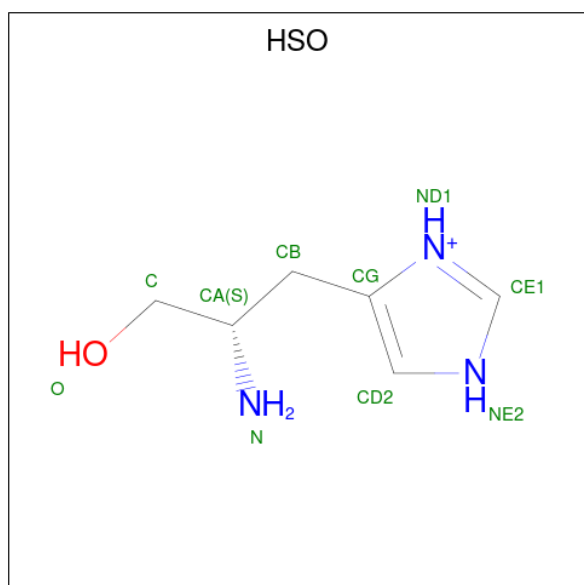
There are 4 unique types of molecules in this entry. The entry contains 14397 atoms, of which 2666 are hydrogens and 0 are deuteriums.

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 HISTIDYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	379	Total	C	H	N	O	S	0	0	0
			3612	1848	674	528	551	11			
1	B	364	Total	C	H	N	O	S	0	0	0
			3455	1768	643	505	528	11			
1	C	387	Total	C	H	N	O	S	0	0	0
			3666	1876	682	536	561	11			
1	D	364	Total	C	H	N	O	S	0	0	0
			3452	1765	643	505	528	11			

- Molecule 2 is L-histidinol (CCD ID: HSO) (formula: C₆H₁₂N₃O).



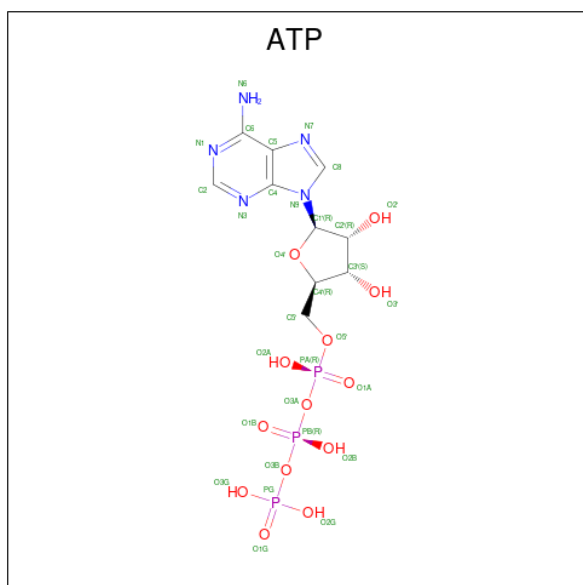
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			13	6	3	3	1		
2	B	1	Total	C	H	N	O	0	0
			13	6	3	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	0	0
			13	6	3	3	1		
2	D	1	Total	C	H	N	O	0	0
			13	6	3	3	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



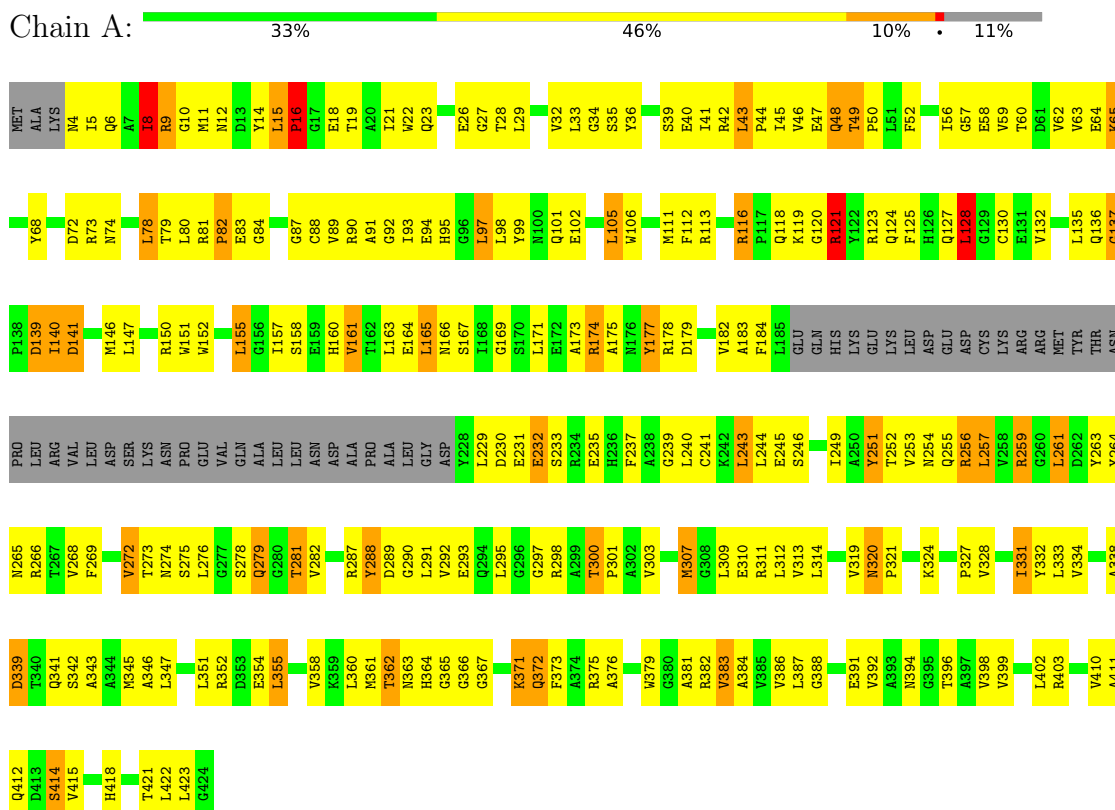
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	O	0	0
			2	2		

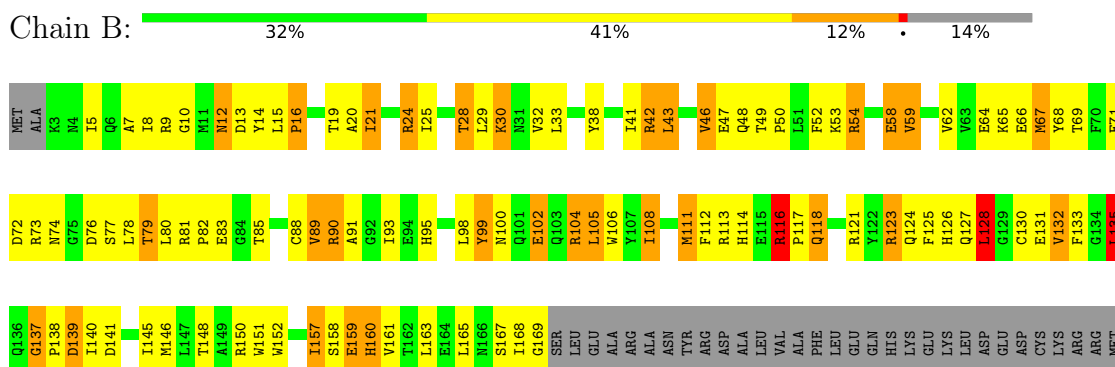
3 Residue-property plots

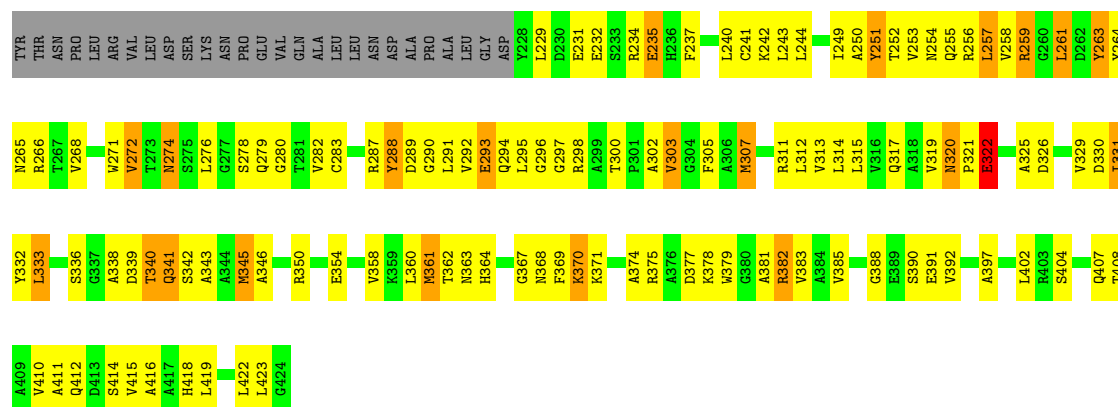
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

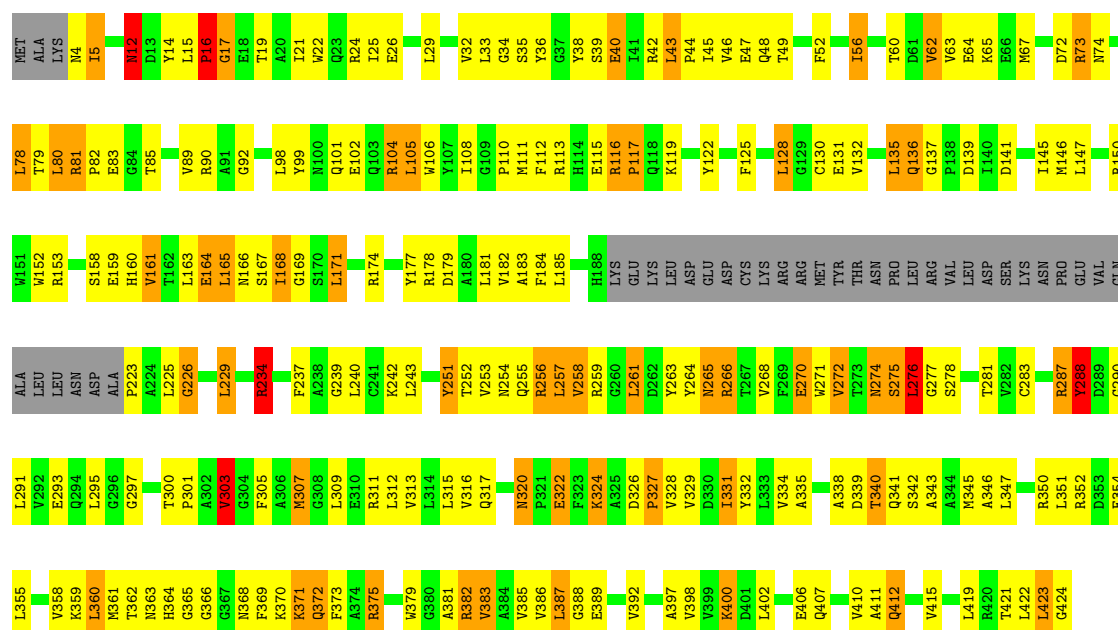


• Molecule 1: HISTIDYL-TRNA SYNTHETASE

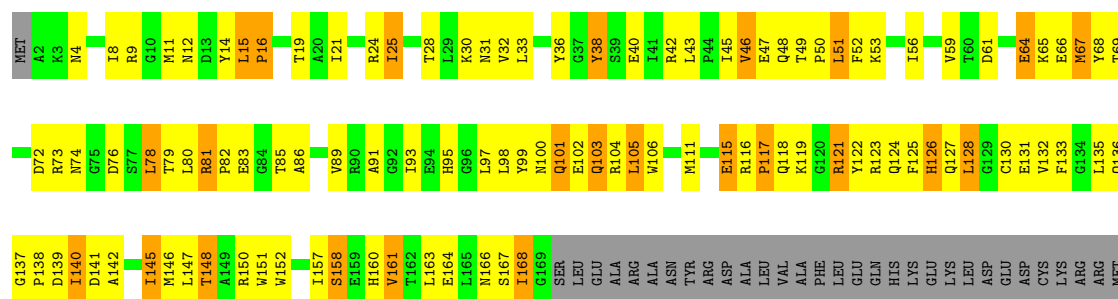
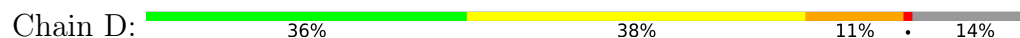




• Molecule 1: HISTIDYL-TRNA SYNTHETASE



• Molecule 1: HISTIDYL-TRNA SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.90Å 107.30Å 107.20Å 114.10° 97.40° 90.00°	Depositor
Resolution (Å)	13.00 – 2.80 13.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	64.0 (13.00-2.80) 68.0 (13.00-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.35 (at 2.61Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.249 , 0.348 0.241 , 0.264	Depositor DCC
R_{free} test set	1585 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14397	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HSO, ATP

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	0.92	0/2991	1.30	34/4046 (0.8%)
1	B	0.95	3/2863 (0.1%)	1.32	33/3873 (0.9%)
1	C	0.92	2/3037 (0.1%)	1.27	28/4109 (0.7%)
1	D	0.93	2/2860 (0.1%)	1.27	27/3869 (0.7%)
All	All	0.93	7/11751 (0.1%)	1.29	122/15897 (0.8%)

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
1	B	0	1
1	C	0	2
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	25	ILE	CA-CB	-7.55	1.44	1.54
1	C	303	VAL	CA-CB	-7.17	1.48	1.55
1	B	59	VAL	CA-CB	5.95	1.62	1.54
1	D	328	VAL	CA-CB	5.80	1.62	1.54
1	C	307	MET	SD-CE	5.80	1.94	1.79
1	B	361	MET	SD-CE	-5.56	1.65	1.79
1	B	62	VAL	CA-CB	5.29	1.60	1.54

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ARG	CA-C-N	12.71	135.73	119.84
1	B	116	ARG	C-N-CA	12.71	135.73	119.84
1	C	43	LEU	CA-C-N	12.20	132.33	119.89
1	C	43	LEU	C-N-CA	12.20	132.33	119.89
1	A	43	LEU	CA-C-N	10.77	130.85	119.76
1	A	43	LEU	C-N-CA	10.77	130.85	119.76
1	C	81	ARG	N-CA-C	10.57	122.57	109.57
1	A	320	ASN	CA-C-N	10.08	132.44	119.84
1	A	320	ASN	C-N-CA	10.08	132.44	119.84
1	B	320	ASN	CA-C-N	9.93	132.25	119.84
1	B	320	ASN	C-N-CA	9.93	132.25	119.84
1	D	43	LEU	CA-C-N	9.21	129.26	119.78
1	D	43	LEU	C-N-CA	9.21	129.26	119.78
1	B	43	LEU	CA-C-N	8.85	128.61	119.76
1	B	43	LEU	C-N-CA	8.85	128.61	119.76
1	D	117	PRO	N-CA-C	8.59	124.76	111.11
1	A	128	LEU	N-CA-C	-8.56	94.95	108.90
1	B	300	THR	CA-C-N	-8.38	112.23	120.52
1	B	300	THR	C-N-CA	-8.38	112.23	120.52
1	D	282	VAL	N-CA-C	-8.38	105.08	112.12
1	C	12	ASN	N-CA-C	8.36	121.83	110.55
1	B	128	LEU	N-CA-C	-8.05	95.78	108.90
1	A	137	GLY	CA-C-N	7.98	128.06	119.28
1	A	137	GLY	C-N-CA	7.98	128.06	119.28
1	D	81	ARG	N-CA-C	7.94	119.34	109.57
1	D	128	LEU	N-CA-C	-7.72	96.32	108.90
1	A	56	ILE	N-CA-C	7.66	118.44	110.62
1	C	290	GLY	N-CA-C	7.55	122.98	114.67
1	A	183	ALA	N-CA-C	-7.46	102.84	110.97
1	B	326	ASP	CA-C-N	-7.43	110.56	119.84
1	B	326	ASP	C-N-CA	-7.43	110.56	119.84
1	D	279	GLN	N-CA-C	-7.40	104.28	113.38
1	C	65	LYS	N-CA-C	7.37	121.99	112.41
1	B	65	LYS	N-CA-C	7.27	122.26	112.88
1	B	282	VAL	CB-CA-C	-7.17	104.63	111.44
1	D	116	ARG	CA-C-N	7.16	127.19	119.89
1	D	116	ARG	C-N-CA	7.16	127.19	119.89
1	B	322	GLU	N-CA-C	-7.04	103.21	111.03
1	B	102	GLU	N-CA-C	-6.98	98.35	109.59
1	A	279	GLN	N-CA-C	-6.91	104.88	113.38
1	D	277	GLY	N-CA-C	-6.77	104.10	112.77
1	B	116	ARG	C-N-CD	-6.76	97.30	125.00
1	A	12	ASN	N-CA-C	6.72	120.46	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	282	VAL	N-CA-C	-6.67	105.83	111.56
1	D	65	LYS	N-CA-C	6.62	121.41	112.88
1	C	128	LEU	N-CA-C	-6.44	97.92	108.41
1	A	282	VAL	CB-CA-C	-6.44	104.15	111.55
1	D	250	ALA	N-CA-C	6.40	118.59	108.67
1	A	65	LYS	N-CA-C	6.40	121.96	112.94
1	C	223	PRO	N-CA-CB	6.29	109.91	103.00
1	C	303	VAL	CB-CA-C	-6.25	103.11	111.80
1	A	164	GLU	N-CA-C	-6.16	99.66	109.76
1	C	300	THR	N-CA-C	-6.15	100.17	108.11
1	D	102	GLU	N-CA-C	-6.08	99.78	109.76
1	D	66	GLU	N-CA-C	6.07	121.73	113.97
1	B	28	THR	N-CA-C	-6.03	104.40	110.97
1	B	123	ARG	N-CA-C	-6.02	104.08	112.45
1	B	279	GLN	N-CA-C	-6.01	98.00	110.80
1	D	262	ASP	N-CA-C	5.92	120.12	113.02
1	A	300	THR	CA-C-N	-5.89	114.53	120.31
1	A	300	THR	C-N-CA	-5.89	114.53	120.31
1	D	36	TYR	N-CA-C	5.89	120.47	113.28
1	C	49	THR	CA-C-N	-5.88	112.81	119.28
1	C	49	THR	C-N-CA	-5.88	112.81	119.28
1	D	291	LEU	N-CA-C	5.76	119.13	111.75
1	B	289	ASP	N-CA-C	5.68	117.56	111.36
1	C	104	ARG	N-CA-C	-5.68	99.02	108.34
1	A	253	VAL	CB-CA-C	-5.68	105.10	111.23
1	B	53	LYS	N-CA-C	-5.67	104.74	111.03
1	D	329	VAL	N-CA-C	5.67	116.64	108.48
1	A	58	GLU	N-CA-C	5.65	117.12	111.07
1	D	282	VAL	CB-CA-C	-5.64	105.38	110.91
1	B	66	GLU	N-CA-C	5.62	121.16	113.97
1	B	135	LEU	N-CA-C	5.62	117.68	108.52
1	C	17	GLY	N-CA-C	5.62	119.69	112.83
1	D	290	GLY	N-CA-C	5.60	120.88	113.37
1	C	145	ILE	N-CA-C	-5.58	105.07	110.42
1	B	329	VAL	N-CA-C	5.46	117.25	108.85
1	A	289	ASP	N-CA-C	5.45	117.22	111.28
1	A	320	ASN	C-N-CD	-5.44	102.68	125.00
1	A	290	GLY	N-CA-C	5.43	121.39	114.66
1	A	87	GLY	N-CA-C	-5.43	106.22	112.73
1	B	296	GLY	N-CA-C	5.41	124.88	116.01
1	A	121	ARG	N-CA-C	5.39	118.90	110.32
1	A	177	TYR	N-CA-C	-5.39	107.72	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	ALA	N-CA-C	5.38	117.02	108.67
1	B	290	GLY	N-CA-C	5.38	121.33	114.66
1	B	160	HIS	N-CA-C	5.33	116.70	110.41
1	D	401	ASP	N-CA-C	-5.32	100.06	108.73
1	C	62	VAL	CB-CA-C	-5.32	105.16	111.81
1	C	327	PRO	N-CA-C	-5.30	103.51	111.57
1	A	49	THR	CA-C-N	-5.29	114.16	119.56
1	A	49	THR	C-N-CA	-5.29	114.16	119.56
1	C	164	GLU	N-CA-C	-5.29	101.09	109.76
1	C	375	ARG	N-CA-C	-5.25	105.56	111.28
1	A	102	GLU	N-CA-C	-5.24	101.15	109.59
1	D	320	ASN	CA-C-N	5.24	126.39	119.84
1	D	320	ASN	C-N-CA	5.24	126.39	119.84
1	B	253	VAL	CB-CA-C	-5.23	105.58	111.23
1	C	56	ILE	N-CA-C	5.21	115.98	110.72
1	B	111	MET	N-CA-C	-5.21	101.45	109.52
1	A	355	LEU	CA-C-N	-5.19	114.64	120.14
1	A	355	LEU	C-N-CA	-5.19	114.64	120.14
1	A	272	VAL	N-CA-C	5.17	115.92	108.48
1	D	406	GLU	N-CA-C	5.14	116.56	109.15
1	A	182	VAL	N-CA-C	5.14	115.86	110.62
1	A	282	VAL	N-CA-C	-5.11	107.42	111.81
1	C	265	ASN	CA-C-N	-5.11	116.36	122.44
1	C	265	ASN	C-N-CA	-5.11	116.36	122.44
1	C	135	LEU	N-CA-C	5.09	117.00	107.99
1	A	339	ASP	N-CA-C	5.07	119.42	113.23
1	B	104	ARG	N-CA-C	-5.07	100.02	108.34
1	C	258	VAL	N-CA-C	-5.07	100.60	108.86
1	B	258	VAL	N-CA-C	-5.06	101.06	108.85
1	C	419	LEU	N-CA-C	-5.06	105.66	111.07
1	C	234	ARG	N-CA-C	-5.05	105.68	111.14
1	D	240	LEU	N-CA-C	-5.05	104.77	112.04
1	C	226	GLY	N-CA-C	-5.04	101.22	113.18
1	C	272	VAL	N-CA-C	5.04	116.55	108.89
1	D	326	ASP	CA-C-N	-5.04	113.55	119.84
1	D	326	ASP	C-N-CA	-5.04	113.55	119.84
1	A	119	LYS	N-CA-C	-5.03	105.27	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	99	TYR	Sidechain
1	C	122	TYR	Sidechain
1	C	288	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	2938	674	2899	221	0
1	B	2812	643	2768	231	0
1	C	2984	682	2932	223	0
1	D	2809	643	2762	237	0
2	A	10	3	11	0	0
2	B	10	3	11	1	0
2	C	10	3	11	2	0
2	D	10	3	11	0	0
3	A	31	3	12	3	0
3	B	31	3	12	11	0
3	C	31	3	12	8	0
3	D	31	3	12	11	0
4	A	13	0	0	0	0
4	B	5	0	0	1	0
4	C	4	0	0	0	0
4	D	2	0	0	0	0
All	All	11731	2666	11453	867	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 37.

All (867) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:MET:HE3	1:B:79:THR:HG21	1.16	1.08
1:C:67:MET:HE3	1:C:79:THR:HG21	1.33	1.07
1:A:136:GLN:HG2	1:A:301:PRO:HG2	1.34	1.05
1:A:120:GLY:HA3	1:A:279:GLN:HG2	1.38	1.03
1:C:350:ARG:HH22	1:C:412:GLN:HG2	1.19	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ARG:NH1	3:B:452:ATP:H2'	1.76	1.00
1:C:370:LYS:HE2	1:C:370:LYS:HA	1.43	1.00
1:B:311:ARG:CZ	3:B:452:ATP:H2'	1.93	0.98
1:A:382:ARG:HG2	1:A:403:ARG:HH21	1.30	0.96
1:C:311:ARG:NH2	3:C:452:ATP:H2'	1.78	0.96
1:C:15:LEU:HD22	1:D:97:LEU:HD11	1.45	0.95
1:C:46:VAL:HG23	1:D:8:ILE:HD12	1.51	0.92
1:D:33:LEU:HD23	1:D:147:LEU:HD11	1.53	0.91
1:D:46:VAL:HG13	1:D:80:LEU:HD12	1.53	0.90
1:C:46:VAL:HG12	1:C:80:LEU:HD12	1.53	0.90
1:D:293:GLU:HA	1:D:297:GLY:O	1.71	0.90
1:A:32:VAL:HG13	1:A:150:ARG:HD2	1.50	0.90
1:A:97:LEU:HD11	1:B:15:LEU:HD12	1.52	0.89
1:C:259:ARG:HG3	1:C:259:ARG:HH11	1.37	0.89
1:C:14:TYR:HB2	1:D:42:ARG:HB2	1.55	0.89
1:A:178:ARG:HG3	1:A:178:ARG:HH11	1.37	0.87
1:D:15:LEU:HD22	1:D:15:LEU:H	1.36	0.87
1:C:331:ILE:HB	1:C:360:LEU:HD12	1.57	0.86
1:C:400:LYS:HG2	1:C:407:GLN:HB3	1.55	0.86
1:A:371:LYS:HE2	1:A:375:ARG:HH21	1.41	0.85
1:B:265:ASN:ND2	1:B:266:ARG:HE	1.73	0.85
1:A:22:TRP:O	1:A:26:GLU:HG3	1.77	0.85
1:C:311:ARG:HH21	3:C:452:ATP:C2'	1.89	0.85
1:C:105:LEU:HD23	1:C:131:GLU:O	1.78	0.84
1:B:141:ASP:HB2	1:B:240:LEU:HD13	1.60	0.84
1:B:382:ARG:HG3	1:B:382:ARG:HH11	1.40	0.84
1:B:46:VAL:HG13	1:B:80:LEU:HD12	1.60	0.83
1:D:130:CYS:SG	1:D:305:PHE:CE2	2.72	0.83
1:A:388:GLY:O	1:A:392:VAL:HG23	1.79	0.82
1:A:14:TYR:HB2	1:B:42:ARG:HB2	1.58	0.82
1:D:234:ARG:HG2	1:D:234:ARG:HH11	1.42	0.82
1:C:256:ARG:HD2	1:C:256:ARG:O	1.80	0.82
1:A:261:LEU:HD23	1:A:264:TYR:HE2	1.43	0.81
1:C:42:ARG:HB2	1:D:14:TYR:HB2	1.62	0.81
1:A:382:ARG:HG2	1:A:403:ARG:NH2	1.94	0.81
1:C:322:GLU:HG3	1:C:324:LYS:HE3	1.63	0.81
1:B:167:SER:HA	1:B:266:ARG:O	1.80	0.81
1:C:104:ARG:HG2	1:C:132:VAL:HG13	1.61	0.81
1:B:382:ARG:HG3	1:B:382:ARG:NH1	1.93	0.80
1:D:332:TYR:CE1	1:D:363:ASN:HB2	2.17	0.80
1:D:67:MET:HE3	1:D:79:THR:HG21	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ARG:HH22	3:D:452:ATP:PG	2.05	0.79
1:B:278:SER:CA	1:B:311:ARG:HB3	2.12	0.79
1:C:67:MET:CE	1:C:79:THR:HG21	2.13	0.79
1:A:259:ARG:HG3	1:A:259:ARG:HH11	1.49	0.78
1:C:168:ILE:HG22	1:C:265:ASN:O	1.84	0.78
1:D:412:GLN:HA	1:D:415:VAL:HG23	1.66	0.78
1:C:311:ARG:NH2	3:C:452:ATP:C2'	2.46	0.78
1:D:383:VAL:HG11	1:D:419:LEU:CD2	2.14	0.78
1:B:21:ILE:O	1:B:25:ILE:HG13	1.83	0.77
1:C:334:VAL:HG11	1:C:373:PHE:HE1	1.48	0.77
1:D:142:ALA:HA	1:D:145:ILE:HD12	1.65	0.77
1:C:350:ARG:NH2	1:C:412:GLN:HG2	1.98	0.77
1:C:287:ARG:HA	1:C:303:VAL:HG12	1.67	0.77
1:D:241:CYS:SG	1:D:251:TYR:CZ	2.76	0.77
1:A:52:PHE:CE1	1:A:82:PRO:HD2	2.20	0.76
1:C:25:ILE:HD13	1:C:316:VAL:HG21	1.66	0.76
1:A:345:MET:HG3	1:A:362:THR:HG21	1.67	0.75
1:C:169:GLY:HA3	1:C:229:LEU:CD2	2.16	0.75
1:A:310:GLU:O	1:A:314:LEU:HD13	1.86	0.75
1:D:328:VAL:HG22	1:D:329:VAL:HG23	1.69	0.75
1:A:352:ARG:HB2	1:B:150:ARG:HH12	1.49	0.75
1:C:168:ILE:HD11	1:C:258:VAL:HG22	1.70	0.74
1:C:334:VAL:HG21	1:C:373:PHE:CE1	2.22	0.74
1:C:163:LEU:HD23	1:C:271:TRP:CE2	2.22	0.74
1:C:423:LEU:HD12	1:C:424:GLY:O	1.87	0.74
1:A:9:ARG:H	1:A:9:ARG:NE	1.85	0.74
1:C:115:GLU:O	1:C:117:PRO:HD3	1.88	0.73
1:A:105:LEU:HD23	1:A:105:LEU:N	2.03	0.73
1:C:397:ALA:HB2	1:C:412:GLN:NE2	2.04	0.73
2:C:451:HSO:H1	3:C:452:ATP:O1A	1.89	0.73
1:C:383:VAL:HG11	1:C:422:LEU:HD13	1.70	0.73
1:B:311:ARG:NH1	3:B:452:ATP:C2'	2.52	0.73
1:B:234:ARG:HH21	1:B:237:PHE:HD2	1.36	0.73
1:C:167:SER:HA	1:C:266:ARG:O	1.88	0.73
1:D:104:ARG:C	1:D:105:LEU:HG	2.11	0.72
1:B:38:TYR:CE1	1:B:104:ARG:HD3	2.25	0.72
1:B:67:MET:CE	1:B:79:THR:HG21	2.09	0.72
1:C:178:ARG:HA	1:C:181:LEU:HB3	1.71	0.72
1:A:146:MET:HE1	1:B:345:MET:SD	2.29	0.72
1:C:136:GLN:HG3	1:C:301:PRO:HG2	1.72	0.72
1:D:141:ASP:HB2	1:D:240:LEU:HD13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:HD3	1:B:325:ALA:HB1	1.70	0.72
1:C:254:ASN:OD1	1:C:256:ARG:HG3	1.89	0.72
1:D:265:ASN:ND2	1:D:289:ASP:H	1.88	0.72
1:A:414:SER:O	1:A:418:HIS:HD2	1.73	0.71
1:C:169:GLY:HA3	1:C:229:LEU:HD21	1.72	0.71
1:A:160:HIS:O	1:A:161:VAL:HG13	1.90	0.71
1:B:255:GLN:HA	1:B:255:GLN:OE1	1.89	0.71
1:B:293:GLU:HA	1:B:297:GLY:O	1.91	0.71
1:D:73:ARG:HH11	1:D:73:ARG:HG3	1.56	0.71
1:B:114:HIS:CE1	1:B:123:ARG:HH21	2.08	0.71
1:C:371:LYS:HD2	1:C:375:ARG:HE	1.56	0.71
1:D:244:LEU:HD12	1:D:251:TYR:HD2	1.55	0.71
1:A:256:ARG:HD2	1:A:256:ARG:O	1.91	0.70
1:C:364:HIS:HD2	1:D:104:ARG:NH2	1.89	0.70
1:C:12:ASN:H	1:C:12:ASN:ND2	1.86	0.70
1:C:388:GLY:O	1:C:392:VAL:HG23	1.90	0.70
1:D:333:LEU:HD13	1:D:348:ALA:HB2	1.74	0.70
1:B:28:THR:O	1:B:32:VAL:HG23	1.92	0.70
1:D:28:THR:O	1:D:32:VAL:HG23	1.92	0.70
1:A:9:ARG:H	1:A:9:ARG:HE	1.40	0.70
1:C:324:LYS:H	1:C:324:LYS:HD2	1.57	0.69
1:C:352:ARG:HB2	1:D:150:ARG:HH12	1.56	0.69
1:D:264:TYR:HA	1:D:287:ARG:O	1.92	0.69
1:A:42:ARG:HB2	1:B:14:TYR:HB2	1.72	0.69
1:C:89:VAL:HG21	1:C:291:LEU:HD22	1.73	0.69
1:A:92:GLY:HA3	1:A:98:LEU:HD11	1.74	0.69
1:D:257:LEU:HD23	1:D:268:VAL:HG12	1.73	0.69
1:A:244:LEU:HD12	1:A:249:ILE:HB	1.74	0.68
1:A:361:MET:HE2	1:B:104:ARG:HD2	1.75	0.68
1:B:332:TYR:CE1	1:B:363:ASN:HB2	2.28	0.68
1:B:331:ILE:HD11	1:B:423:LEU:HD11	1.74	0.68
1:A:239:GLY:O	1:A:243:LEU:HD13	1.93	0.68
1:C:5:ILE:HD12	1:D:51:LEU:HG	1.75	0.68
1:B:264:TYR:HA	1:B:287:ARG:O	1.92	0.68
1:B:121:ARG:HH12	3:B:452:ATP:PG	2.16	0.68
1:D:307:MET:SD	1:D:312:LEU:HD22	2.33	0.68
1:D:308:GLY:O	1:D:311:ARG:HG2	1.92	0.68
1:D:257:LEU:HD11	1:D:270:GLU:OE2	1.93	0.68
1:A:345:MET:HB3	1:B:146:MET:HE1	1.76	0.68
1:C:52:PHE:CE2	1:C:82:PRO:HD2	2.28	0.68
1:C:234:ARG:NH1	1:C:237:PHE:HD2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:THR:O	1:A:64:GLU:HG3	1.94	0.68
1:D:111:MET:HB2	1:D:125:PHE:CE1	2.29	0.67
1:D:235:GLU:HG2	1:D:236:HIS:N	2.09	0.67
1:B:52:PHE:CE1	1:B:82:PRO:HD2	2.28	0.67
1:C:105:LEU:O	1:C:130:CYS:HB2	1.94	0.67
1:D:167:SER:HA	1:D:266:ARG:O	1.95	0.67
1:A:332:TYR:HD2	1:A:376:ALA:HB2	1.59	0.67
1:C:111:MET:HB2	1:C:125:PHE:CE1	2.29	0.67
1:A:178:ARG:HG3	1:A:179:ASP:N	2.08	0.66
1:C:272:VAL:HG12	1:C:281:THR:HG22	1.76	0.66
1:B:382:ARG:HH11	1:B:382:ARG:CG	2.09	0.66
1:B:151:TRP:CZ3	1:B:307:MET:HE2	2.31	0.66
1:C:311:ARG:HH21	3:C:452:ATP:C1'	2.09	0.66
1:C:44:PRO:HA	1:D:124:GLN:HE22	1.61	0.66
1:B:388:GLY:O	1:B:392:VAL:HG23	1.96	0.65
1:B:91:ALA:O	1:B:95:HIS:HD2	1.79	0.65
1:D:259:ARG:HB2	1:D:264:TYR:CD2	2.31	0.65
1:A:171:LEU:HD13	1:A:174:ARG:HH12	1.60	0.65
1:B:383:VAL:HG11	1:B:419:LEU:HD21	1.79	0.65
1:D:47:GLU:HB2	1:D:52:PHE:CE2	2.32	0.65
1:D:121:ARG:NH2	3:D:452:ATP:PG	2.70	0.65
1:A:373:PHE:O	1:A:376:ALA:HB3	1.97	0.65
1:C:22:TRP:O	1:C:26:GLU:HG3	1.97	0.65
1:A:97:LEU:N	1:A:97:LEU:HD23	2.12	0.65
1:D:168:ILE:HG22	1:D:265:ASN:O	1.96	0.65
1:A:60:THR:HG22	1:A:62:VAL:H	1.61	0.65
1:C:160:HIS:O	1:C:161:VAL:HG13	1.97	0.64
1:A:309:LEU:O	1:A:313:VAL:HG23	1.97	0.64
1:B:9:ARG:HE	1:B:116:ARG:HH22	1.45	0.64
1:B:38:TYR:N	1:B:38:TYR:HD1	1.96	0.64
1:B:237:PHE:O	1:B:241:CYS:SG	2.53	0.64
1:B:105:LEU:O	1:B:130:CYS:HB2	1.97	0.64
1:A:113:ARG:HG3	1:A:125:PHE:HE2	1.62	0.64
1:C:347:LEU:HG	1:C:351:LEU:CD1	2.28	0.64
1:C:271:TRP:HB2	1:C:283:CYS:HB3	1.80	0.64
1:C:36:TYR:HE1	1:C:150:ARG:HD2	1.62	0.64
1:D:263:TYR:HD2	1:D:291:LEU:HD13	1.63	0.64
1:D:311:ARG:HG3	1:D:311:ARG:HH11	1.63	0.64
1:C:92:GLY:HA3	1:C:98:LEU:HD11	1.80	0.64
1:C:309:LEU:O	1:C:313:VAL:HG23	1.97	0.64
1:B:74:ASN:HB3	1:B:76:ASP:OD1	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:VAL:HG11	1:B:419:LEU:CD2	2.28	0.63
1:B:58:GLU:CD	1:B:58:GLU:H	2.06	0.63
1:C:116:ARG:HH11	1:C:116:ARG:HG3	1.62	0.63
1:A:165:LEU:HD12	1:A:166:ASN:H	1.63	0.63
1:C:40:GLU:HB2	1:C:106:TRP:CZ2	2.34	0.63
1:A:141:ASP:HB2	1:A:240:LEU:HD13	1.80	0.63
1:D:135:LEU:O	1:D:287:ARG:NH2	2.32	0.63
1:B:89:VAL:HG21	1:B:291:LEU:HD21	1.80	0.63
1:B:152:TRP:CD1	1:B:161:VAL:HG21	2.34	0.63
1:A:33:LEU:HD23	1:A:147:LEU:HD11	1.80	0.62
1:B:135:LEU:HD23	1:B:140:ILE:HD13	1.81	0.62
1:C:352:ARG:CB	1:D:150:ARG:HH12	2.11	0.62
1:D:127:GLN:NE2	3:D:452:ATP:H5'1	2.14	0.62
1:C:52:PHE:HB3	1:C:56:ILE:HD12	1.80	0.62
1:D:133:PHE:HE1	1:D:288:TYR:HH	1.46	0.62
1:A:45:ILE:HG12	1:B:124:GLN:HE22	1.63	0.62
1:A:175:ALA:O	1:A:178:ARG:HG2	1.99	0.62
1:B:21:ILE:H	1:B:21:ILE:HD12	1.64	0.62
1:B:265:ASN:ND2	1:B:266:ARG:NE	2.46	0.62
1:D:15:LEU:H	1:D:15:LEU:CD2	2.11	0.62
1:B:10:GLY:HA3	1:B:123:ARG:HG2	1.80	0.62
1:D:105:LEU:O	1:D:130:CYS:HB2	1.99	0.62
1:D:49:THR:O	1:D:53:LYS:HG3	2.00	0.62
1:A:178:ARG:HG3	1:A:179:ASP:H	1.63	0.62
1:B:343:ALA:O	1:B:346:ALA:HB3	2.00	0.62
1:D:259:ARG:NH2	3:D:452:ATP:O1A	2.33	0.62
1:A:163:LEU:HD21	1:A:165:LEU:HD22	1.81	0.62
1:A:381:ALA:O	1:A:402:LEU:HD12	1.99	0.62
1:B:361:MET:HE1	1:B:379:TRP:CE2	2.35	0.61
1:D:72:ASP:HB2	1:D:78:LEU:CD2	2.30	0.61
1:C:259:ARG:NH2	3:C:452:ATP:O1A	2.32	0.61
1:D:157:ILE:HG22	1:D:319:VAL:CG1	2.30	0.61
1:D:259:ARG:HG2	1:D:268:VAL:HG13	1.82	0.61
1:B:38:TYR:N	1:B:38:TYR:CD1	2.68	0.61
1:D:412:GLN:HA	1:D:415:VAL:CG2	2.31	0.61
1:A:383:VAL:HG11	1:A:422:LEU:HD13	1.83	0.61
1:C:287:ARG:O	1:C:288:TYR:HB3	1.98	0.61
1:B:125:PHE:HE1	1:B:127:GLN:HG3	1.66	0.61
1:C:347:LEU:HG	1:C:351:LEU:HD12	1.83	0.61
1:D:30:LYS:HZ3	1:D:30:LYS:HB2	1.66	0.61
1:B:68:TYR:HB2	1:B:80:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:TRP:CE3	1:B:307:MET:HE2	2.35	0.60
1:C:29:LEU:HD11	1:C:312:LEU:CD2	2.31	0.60
1:B:141:ASP:O	1:B:145:ILE:HD12	2.01	0.60
1:B:251:TYR:H	1:B:251:TYR:HD1	1.47	0.60
1:B:418:HIS:O	1:B:422:LEU:HD23	2.01	0.60
1:D:45:ILE:O	1:D:81:ARG:HG2	2.01	0.60
1:B:168:ILE:HG13	1:B:265:ASN:O	2.02	0.60
1:A:259:ARG:HH11	1:A:259:ARG:CG	2.14	0.60
1:A:259:ARG:NH2	3:A:452:ATP:O1A	2.34	0.60
1:B:106:TRP:HA	1:B:130:CYS:HA	1.82	0.60
1:C:147:LEU:HD23	1:C:147:LEU:C	2.26	0.60
1:C:259:ARG:HH11	1:C:259:ARG:CG	2.11	0.60
1:C:334:VAL:HG11	1:C:373:PHE:CE1	2.32	0.60
1:A:251:TYR:HD1	1:A:251:TYR:H	1.50	0.60
1:C:340:THR:HG23	1:C:387:LEU:HD13	1.83	0.60
1:A:165:LEU:HD13	1:A:269:PHE:HB3	1.83	0.60
1:C:277:GLY:O	1:C:311:ARG:HG2	2.02	0.60
1:A:298:ARG:HG3	1:A:298:ARG:HH11	1.66	0.59
1:A:29:LEU:HD13	1:A:128:LEU:HD23	1.83	0.59
1:C:38:TYR:CE2	1:C:104:ARG:HB3	2.37	0.59
1:C:293:GLU:HA	1:C:297:GLY:O	2.03	0.59
1:D:279:GLN:H	1:D:311:ARG:NH2	1.99	0.59
1:B:333:LEU:HD13	1:B:385:VAL:O	2.03	0.59
1:C:226:GLY:O	1:C:229:LEU:HB2	2.02	0.59
1:D:141:ASP:HB2	1:D:240:LEU:CD1	2.32	0.59
1:B:12:ASN:H	1:B:12:ASN:ND2	1.99	0.59
1:C:368:ASN:OD1	1:C:370:LYS:HB2	2.03	0.59
1:B:15:LEU:O	1:B:19:THR:HG23	2.02	0.59
1:C:72:ASP:HB2	1:C:78:LEU:CD2	2.32	0.59
1:C:72:ASP:HB2	1:C:78:LEU:HD22	1.84	0.59
1:A:165:LEU:HD23	1:A:251:TYR:HD2	1.68	0.59
1:A:83:GLU:HG3	1:A:84:GLY:N	2.13	0.59
1:B:118:GLN:HA	1:B:118:GLN:NE2	2.17	0.59
1:C:345:MET:HG3	1:C:362:THR:HG21	1.84	0.59
1:C:345:MET:HE3	1:D:146:MET:HE1	1.83	0.59
1:D:136:GLN:HE22	1:D:266:ARG:HH12	1.50	0.59
1:A:22:TRP:HH2	1:A:310:GLU:HG3	1.68	0.59
1:C:105:LEU:N	1:C:105:LEU:CD2	2.66	0.59
1:D:157:ILE:HG22	1:D:319:VAL:HG11	1.84	0.59
1:A:293:GLU:HA	1:A:297:GLY:O	2.02	0.59
1:A:355:LEU:O	1:A:358:VAL:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ASP:O	1:D:145:ILE:HG13	2.02	0.58
1:A:163:LEU:HD23	1:A:251:TYR:HB3	1.85	0.58
1:C:104:ARG:HG2	1:C:132:VAL:CG1	2.33	0.58
1:D:99:TYR:O	1:D:101:GLN:HG2	2.02	0.58
1:A:167:SER:HA	1:A:266:ARG:O	2.02	0.58
1:C:313:VAL:HG12	1:C:317:GLN:NE2	2.17	0.58
1:D:21:ILE:O	1:D:25:ILE:HG13	2.03	0.58
1:D:332:TYR:CZ	1:D:363:ASN:HB2	2.38	0.58
1:B:21:ILE:HD12	1:B:21:ILE:N	2.19	0.58
1:B:278:SER:C	1:B:280:GLY:H	2.10	0.58
1:C:291:LEU:HD21	1:C:295:LEU:HD22	1.84	0.58
1:B:234:ARG:NH2	1:B:237:PHE:HD2	2.01	0.58
1:A:254:ASN:OD1	1:A:256:ARG:HG3	2.03	0.58
1:B:331:ILE:HD12	1:B:331:ILE:N	2.19	0.58
1:D:67:MET:CE	1:D:79:THR:HG21	2.33	0.58
1:A:147:LEU:HD23	1:A:147:LEU:O	2.04	0.58
1:A:173:ALA:O	1:A:177:TYR:HB2	2.04	0.58
1:D:38:TYR:N	1:D:38:TYR:CD1	2.72	0.58
1:B:320:ASN:C	1:B:322:GLU:H	2.11	0.58
1:B:112:PHE:HA	1:B:123:ARG:O	2.04	0.58
1:D:234:ARG:HH11	1:D:234:ARG:CG	2.14	0.58
1:A:307:MET:SD	1:A:312:LEU:HD22	2.43	0.58
1:D:319:VAL:C	1:D:321:PRO:HD3	2.28	0.58
1:C:259:ARG:HG3	1:C:259:ARG:NH1	2.15	0.57
1:D:106:TRP:HA	1:D:130:CYS:HA	1.85	0.57
1:C:311:ARG:NH2	3:C:452:ATP:C4	2.72	0.57
1:C:382:ARG:HH11	1:C:382:ARG:HB2	1.69	0.57
1:D:38:TYR:N	1:D:38:TYR:HD1	2.01	0.57
1:C:22:TRP:CE2	1:C:313:VAL:HG21	2.40	0.57
1:B:43:LEU:HD11	1:B:88:CYS:HA	1.86	0.57
1:B:130:CYS:SG	1:B:305:PHE:CE1	2.96	0.57
1:C:345:MET:HE3	1:D:146:MET:SD	2.45	0.57
1:C:174:ARG:HG3	1:C:174:ARG:HH11	1.69	0.57
1:D:265:ASN:HD21	1:D:289:ASP:H	1.50	0.57
1:C:105:LEU:HD23	1:C:105:LEU:N	2.20	0.57
1:C:254:ASN:HD21	1:C:256:ARG:NE	2.02	0.57
1:C:381:ALA:O	1:C:402:LEU:HD12	2.03	0.57
1:B:369:PHE:N	1:B:370:LYS:HZ2	2.03	0.57
1:C:257:LEU:HD11	1:C:270:GLU:HG2	1.87	0.57
1:A:345:MET:HE3	1:B:146:MET:SD	2.45	0.57
1:B:46:VAL:CG1	1:B:80:LEU:HD12	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:LEU:HG	1:C:182:VAL:N	2.19	0.57
1:A:331:ILE:O	1:A:360:LEU:HA	2.05	0.56
1:B:47:GLU:HB2	1:B:52:PHE:HE2	1.70	0.56
1:A:72:ASP:HB2	1:A:78:LEU:HD22	1.86	0.56
1:A:384:ALA:HB2	1:A:402:LEU:HD21	1.85	0.56
1:C:47:GLU:OE2	1:C:90:ARG:HD3	2.05	0.56
1:B:265:ASN:HD21	1:B:266:ARG:HE	1.52	0.56
1:C:182:VAL:HA	1:C:185:LEU:HB2	1.86	0.56
1:C:234:ARG:HH12	1:C:237:PHE:HD2	1.53	0.56
1:C:345:MET:HE3	1:D:146:MET:CE	2.35	0.56
1:A:273:THR:C	1:A:275:SER:H	2.13	0.56
1:B:72:ASP:HB2	1:B:78:LEU:HD11	1.87	0.56
1:B:283:CYS:SG	1:B:305:PHE:HD2	2.29	0.56
1:B:311:ARG:CZ	3:B:452:ATP:C2'	2.77	0.56
1:A:264:TYR:HA	1:A:287:ARG:O	2.06	0.56
1:B:137:GLY:O	1:B:140:ILE:HG22	2.06	0.56
1:B:259:ARG:HG2	1:B:268:VAL:HG13	1.88	0.56
1:D:311:ARG:HD3	3:D:452:ATP:N3	2.20	0.56
1:A:178:ARG:HH11	1:A:178:ARG:CG	2.15	0.56
1:B:89:VAL:HG21	1:B:291:LEU:CD2	2.36	0.56
1:B:141:ASP:HB2	1:B:240:LEU:CD1	2.32	0.56
1:D:164:GLU:HB2	1:D:270:GLU:HG3	1.87	0.56
1:A:163:LEU:HD23	1:A:251:TYR:CB	2.35	0.56
1:A:254:ASN:HD21	1:A:256:ARG:NH2	2.04	0.56
1:C:147:LEU:HD23	1:C:147:LEU:O	2.06	0.56
1:B:261:LEU:HD12	1:B:263:TYR:CZ	2.42	0.55
1:B:287:ARG:O	1:B:288:TYR:HB3	2.06	0.55
1:D:72:ASP:HB2	1:D:78:LEU:HD22	1.88	0.55
1:A:394:ASN:O	1:A:396:THR:HG23	2.07	0.55
1:B:14:TYR:HE2	1:B:126:HIS:HE1	1.54	0.55
1:C:113:ARG:HD2	1:C:125:PHE:CE1	2.41	0.55
1:A:8:ILE:H	1:A:8:ILE:CD1	2.19	0.55
1:C:81:ARG:HD2	1:C:111:MET:SD	2.45	0.55
1:C:166:ASN:HB3	1:C:268:VAL:HG23	1.87	0.55
1:C:313:VAL:HG12	1:C:317:GLN:HE21	1.72	0.55
1:A:382:ARG:HG3	1:A:403:ARG:HE	1.71	0.55
1:C:355:LEU:O	1:C:358:VAL:HG22	2.06	0.55
1:D:121:ARG:NH2	3:D:452:ATP:O2G	2.40	0.55
1:B:283:CYS:SG	1:B:305:PHE:CD2	3.00	0.55
1:D:103:GLN:HG3	1:D:105:LEU:HD21	1.88	0.55
1:A:273:THR:OG1	1:A:275:SER:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:SER:C	1:B:280:GLY:N	2.64	0.55
1:C:99:TYR:O	1:C:101:GLN:HG3	2.07	0.55
1:C:345:MET:SD	1:C:364:HIS:HE1	2.29	0.55
1:A:95:HIS:HB2	1:A:97:LEU:HD21	1.89	0.54
1:A:361:MET:SD	1:B:104:ARG:NH1	2.80	0.54
1:D:368:ASN:ND2	1:D:371:LYS:HE3	2.22	0.54
1:B:47:GLU:HB2	1:B:52:PHE:CE2	2.42	0.54
1:B:274:ASN:OD1	1:B:274:ASN:N	2.40	0.54
1:A:171:LEU:H	1:A:171:LEU:HD22	1.72	0.54
1:D:383:VAL:HG12	1:D:384:ALA:N	2.22	0.54
1:A:292:VAL:HG21	1:A:300:THR:HG22	1.89	0.54
1:D:49:THR:HG23	1:D:79:THR:OG1	2.08	0.54
1:D:147:LEU:HD23	1:D:147:LEU:O	2.07	0.54
1:A:178:ARG:HG3	1:A:178:ARG:NH1	2.09	0.54
1:C:33:LEU:HD23	1:C:147:LEU:HD11	1.89	0.54
1:C:225:LEU:O	1:C:229:LEU:HG	2.08	0.54
1:D:166:ASN:HD22	1:D:168:ILE:HD13	1.73	0.53
1:B:69:THR:HA	1:B:78:LEU:O	2.07	0.53
1:D:133:PHE:HE1	1:D:288:TYR:OH	1.91	0.53
1:D:136:GLN:HE22	1:D:266:ARG:NH1	2.05	0.53
1:D:148:THR:O	1:D:151:TRP:HB2	2.08	0.53
1:A:105:LEU:N	1:A:105:LEU:CD2	2.72	0.53
1:A:382:ARG:CG	1:A:403:ARG:HE	2.21	0.53
1:C:46:VAL:HG23	1:D:8:ILE:CD1	2.32	0.53
1:D:83:GLU:C	1:D:111:MET:HE3	2.33	0.53
1:D:141:ASP:CB	1:D:240:LEU:HD13	2.39	0.53
1:D:321:PRO:O	1:D:324:LYS:NZ	2.42	0.53
1:C:169:GLY:HA3	1:C:229:LEU:HD22	1.89	0.53
1:B:288:TYR:O	1:B:288:TYR:CD1	2.62	0.53
1:D:125:PHE:CD2	3:D:452:ATP:C6	2.96	0.53
1:C:234:ARG:NH1	1:C:237:PHE:CD2	2.76	0.53
1:C:335:ALA:HB1	1:C:340:THR:HG21	1.90	0.53
1:D:311:ARG:HG3	1:D:311:ARG:NH1	2.24	0.53
3:B:452:ATP:H8	3:B:452:ATP:O2B	1.92	0.53
1:A:89:VAL:O	1:A:93:ILE:HG13	2.09	0.52
1:A:105:LEU:HD23	1:A:105:LEU:H	1.74	0.52
1:A:174:ARG:HB2	1:A:174:ARG:HH11	1.73	0.52
1:D:168:ILE:HD11	1:D:258:VAL:HG12	1.89	0.52
1:A:45:ILE:HD13	1:A:81:ARG:NH2	2.24	0.52
1:C:328:VAL:HG21	1:C:379:TRP:HE3	1.74	0.52
1:A:72:ASP:C	1:A:74:ASN:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ARG:NH2	1:A:423:LEU:HD22	2.24	0.52
1:B:278:SER:CA	1:B:311:ARG:HD3	2.40	0.52
1:B:312:LEU:HD23	1:B:313:VAL:N	2.24	0.52
1:C:22:TRP:NE1	1:C:313:VAL:HG11	2.24	0.52
1:D:251:TYR:C	1:D:251:TYR:HD1	2.18	0.52
1:B:74:ASN:ND2	1:B:74:ASN:O	2.42	0.52
1:C:106:TRP:HA	1:C:130:CYS:HA	1.92	0.52
1:C:370:LYS:HA	1:C:370:LYS:CE	2.27	0.52
1:A:45:ILE:H	1:B:124:GLN:HE22	1.58	0.52
1:A:375:ARG:O	1:A:379:TRP:CD1	2.62	0.52
1:B:259:ARG:CG	1:B:268:VAL:HG13	2.39	0.52
1:D:21:ILE:HD12	1:D:21:ILE:H	1.74	0.52
1:D:119:LYS:HG3	1:D:122:TYR:OH	2.10	0.52
1:A:174:ARG:HH21	1:A:265:ASN:HA	1.75	0.52
1:A:298:ARG:HG3	1:A:298:ARG:NH1	2.25	0.52
1:D:328:VAL:O	1:D:359:LYS:HD3	2.09	0.52
1:B:412:GLN:HA	1:B:415:VAL:HG23	1.92	0.52
1:C:412:GLN:HA	1:C:415:VAL:HG23	1.91	0.52
1:D:139:ASP:O	1:D:142:ALA:HB3	2.09	0.52
1:A:261:LEU:HD23	1:A:264:TYR:CE2	2.32	0.52
1:A:345:MET:CE	1:B:146:MET:SD	2.98	0.52
1:B:354:GLU:OE1	1:B:416:ALA:HB2	2.09	0.52
1:C:283:CYS:SG	1:C:305:PHE:CD1	3.02	0.52
1:D:91:ALA:O	1:D:95:HIS:HD2	1.92	0.52
1:B:415:VAL:HG12	1:B:419:LEU:HD12	1.91	0.52
1:C:331:ILE:O	1:C:360:LEU:HA	2.10	0.52
1:D:73:ARG:HH11	1:D:73:ARG:CG	2.22	0.52
1:A:410:VAL:HG12	1:A:411:ALA:N	2.24	0.51
1:D:130:CYS:SG	1:D:305:PHE:HE2	2.32	0.51
1:A:422:LEU:O	1:A:422:LEU:HD23	2.10	0.51
1:A:5:ILE:HD12	1:B:54:ARG:NH2	2.25	0.51
1:B:111:MET:HB2	1:B:125:PHE:CE1	2.44	0.51
1:B:332:TYR:CZ	1:B:363:ASN:HB2	2.45	0.51
1:A:136:GLN:HG2	1:A:301:PRO:CG	2.24	0.51
1:A:352:ARG:CB	1:B:150:ARG:HH12	2.22	0.51
1:D:93:ILE:HG12	1:D:297:GLY:HA3	1.92	0.51
1:A:11:MET:HG2	1:A:124:GLN:HB2	1.93	0.51
1:A:332:TYR:CD2	1:A:376:ALA:HB2	2.43	0.51
1:B:89:VAL:HG12	1:B:292:VAL:HG12	1.93	0.51
1:B:410:VAL:HG12	1:B:411:ALA:N	2.24	0.51
1:B:133:PHE:HE1	1:B:288:TYR:OH	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:O	1:B:244:LEU:HD23	2.10	0.51
1:B:370:LYS:CD	1:B:370:LYS:H	2.24	0.51
1:B:371:LYS:O	1:B:375:ARG:HG3	2.11	0.51
1:B:132:VAL:HG21	1:B:140:ILE:HD11	1.93	0.51
1:D:52:PHE:HB2	1:D:67:MET:HE1	1.91	0.51
1:B:311:ARG:HD2	3:B:452:ATP:O2'	2.10	0.51
1:A:28:THR:O	1:A:32:VAL:HG23	2.11	0.51
1:D:311:ARG:NH1	3:D:452:ATP:O2'	2.43	0.51
1:A:241:CYS:O	1:A:245:GLU:HG3	2.11	0.51
1:D:136:GLN:NE2	1:D:266:ARG:HH12	2.08	0.51
1:A:232:GLU:HB2	1:A:266:ARG:NH2	2.26	0.50
1:B:244:LEU:HD12	1:B:249:ILE:HB	1.92	0.50
1:B:287:ARG:HA	1:B:303:VAL:HG13	1.92	0.50
1:D:151:TRP:CZ3	1:D:307:MET:HE2	2.45	0.50
1:D:259:ARG:CB	1:D:264:TYR:CE2	2.94	0.50
1:C:259:ARG:NH1	1:C:264:TYR:CZ	2.79	0.50
1:B:375:ARG:HA	1:B:378:LYS:HG3	1.92	0.50
1:C:165:LEU:O	1:C:253:VAL:HA	2.12	0.50
1:D:93:ILE:HD11	1:D:292:VAL:O	2.11	0.50
1:D:288:TYR:CE1	1:D:302:ALA:HB1	2.46	0.50
1:A:178:ARG:CG	1:A:178:ARG:NH1	2.72	0.50
1:D:130:CYS:SG	1:D:305:PHE:CZ	3.01	0.50
1:D:263:TYR:HB3	1:D:291:LEU:HD12	1.93	0.50
1:A:135:LEU:HD12	1:A:140:ILE:HG12	1.94	0.50
1:A:136:GLN:CG	1:A:301:PRO:HG2	2.24	0.50
1:A:386:VAL:HB	1:A:398:VAL:HB	1.94	0.50
1:D:251:TYR:C	1:D:251:TYR:CD1	2.88	0.50
1:D:388:GLY:O	1:D:392:VAL:HG23	2.12	0.50
1:A:127:GLN:HE21	3:A:452:ATP:H5'1	1.76	0.50
1:A:287:ARG:HG2	1:A:288:TYR:H	1.76	0.50
1:A:383:VAL:HG22	1:A:422:LEU:HD22	1.94	0.50
1:C:152:TRP:HB3	1:C:158:SER:HA	1.92	0.50
1:C:332:TYR:CZ	1:C:363:ASN:HB2	2.46	0.50
1:A:74:ASN:HA	1:D:73:ARG:O	2.12	0.50
1:A:384:ALA:CB	1:A:402:LEU:HD21	2.42	0.50
1:B:169:GLY:H	1:B:229:LEU:HD11	1.77	0.50
1:B:291:LEU:C	1:B:291:LEU:HD23	2.37	0.50
1:D:146:MET:HG3	1:D:249:ILE:HD11	1.93	0.50
1:A:343:ALA:O	1:A:346:ALA:HB3	2.12	0.50
1:A:347:LEU:HD13	1:A:412:GLN:HG2	1.93	0.50
1:B:381:ALA:O	1:B:402:LEU:HD12	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:VAL:HG21	1:C:291:LEU:CD2	2.38	0.50
1:D:383:VAL:HG11	1:D:419:LEU:HD21	1.94	0.50
1:A:40:GLU:HB2	1:A:106:TRP:CZ2	2.46	0.50
1:B:369:PHE:HB2	1:B:370:LYS:NZ	2.27	0.50
1:A:157:ILE:HD12	1:A:157:ILE:O	2.12	0.49
1:A:171:LEU:HA	1:A:174:ARG:HH12	1.77	0.49
1:A:332:TYR:CZ	1:A:363:ASN:HB2	2.47	0.49
1:B:125:PHE:CE1	1:B:127:GLN:HG3	2.47	0.49
1:B:390:SER:HB2	1:B:391:GLU:OE1	2.12	0.49
1:D:265:ASN:OD1	1:D:266:ARG:N	2.45	0.49
1:A:165:LEU:HD12	1:A:166:ASN:N	2.27	0.49
1:B:320:ASN:O	1:B:322:GLU:N	2.45	0.49
1:D:85:THR:O	1:D:89:VAL:HG23	2.12	0.49
1:C:315:LEU:O	1:C:315:LEU:HD12	2.12	0.49
1:D:244:LEU:HD12	1:D:251:TYR:CD2	2.43	0.49
1:D:369:PHE:O	1:D:373:PHE:CD2	2.65	0.49
1:B:121:ARG:NH1	1:B:311:ARG:HH22	2.10	0.49
1:C:350:ARG:HH22	1:C:412:GLN:CG	2.08	0.49
1:C:371:LYS:HD2	1:C:375:ARG:NE	2.27	0.49
1:D:259:ARG:NH1	1:D:264:TYR:OH	2.45	0.49
1:A:367:GLY:O	1:A:372:GLN:NE2	2.45	0.49
1:B:85:THR:OG1	2:B:451:HSO:N	2.45	0.49
1:B:254:ASN:HB3	1:B:257:LEU:HB2	1.95	0.49
1:C:287:ARG:HA	1:C:303:VAL:CG1	2.41	0.49
1:A:120:GLY:C	1:A:311:ARG:HH21	2.21	0.49
1:C:259:ARG:CG	1:C:259:ARG:NH1	2.72	0.49
1:C:410:VAL:HG12	1:C:411:ALA:N	2.27	0.49
1:D:52:PHE:O	1:D:56:ILE:HB	2.11	0.49
1:A:241:CYS:SG	1:A:251:TYR:HE2	2.36	0.49
1:C:343:ALA:O	1:C:346:ALA:HB3	2.12	0.49
1:B:15:LEU:N	1:B:15:LEU:HD22	2.28	0.49
1:D:135:LEU:CD1	1:D:140:ILE:HG12	2.42	0.49
1:D:288:TYR:CE1	1:D:302:ALA:CB	2.96	0.49
1:D:312:LEU:O	1:D:313:VAL:C	2.55	0.49
1:A:8:ILE:H	1:A:8:ILE:HD13	1.78	0.49
1:A:146:MET:CE	1:B:345:MET:SD	3.00	0.49
1:A:287:ARG:NH1	1:A:303:VAL:CG2	2.75	0.49
1:D:74:ASN:HB3	1:D:76:ASP:OD1	2.13	0.49
1:D:152:TRP:HB3	1:D:158:SER:HA	1.95	0.49
1:A:279:GLN:HB2	1:A:311:ARG:NH1	2.29	0.48
1:B:261:LEU:HD12	1:B:263:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:PHE:CB	1:D:67:MET:HE1	2.42	0.48
1:D:265:ASN:OD1	1:D:266:ARG:HD3	2.13	0.48
1:A:8:ILE:CD1	1:A:8:ILE:N	2.75	0.48
1:A:43:LEU:HB3	1:A:44:PRO:HD2	1.95	0.48
1:B:69:THR:HG23	1:B:78:LEU:O	2.14	0.48
1:D:138:PRO:HB2	1:D:240:LEU:HB2	1.95	0.48
1:A:232:GLU:HB2	1:A:266:ARG:HH21	1.78	0.48
1:C:104:ARG:HH22	1:D:364:HIS:HD2	1.60	0.48
1:C:110:PRO:O	1:C:111:MET:HE2	2.13	0.48
1:C:182:VAL:O	1:C:185:LEU:N	2.46	0.48
1:C:335:ALA:HB1	1:C:340:THR:CG2	2.43	0.48
1:D:136:GLN:NE2	1:D:266:ARG:NH1	2.62	0.48
1:A:5:ILE:HG22	1:A:6:GLN:N	2.29	0.48
1:B:9:ARG:HG2	1:B:9:ARG:HH11	1.77	0.48
3:B:452:ATP:O2B	3:B:452:ATP:C8	2.67	0.48
1:C:36:TYR:HB3	1:C:38:TYR:CE1	2.47	0.48
1:D:291:LEU:HD21	1:D:295:LEU:CD1	2.43	0.48
1:B:99:TYR:O	1:B:100:ASN:ND2	2.47	0.48
1:D:115:GLU:O	1:D:117:PRO:HD3	2.12	0.48
1:D:126:HIS:ND1	1:D:126:HIS:N	2.61	0.48
1:C:239:GLY:O	1:C:243:LEU:HG	2.13	0.48
1:D:383:VAL:HG22	1:D:422:LEU:HD13	1.95	0.48
1:A:41:ILE:HG22	1:A:106:TRP:O	2.13	0.48
1:A:89:VAL:HG13	1:A:292:VAL:HG12	1.96	0.48
1:A:147:LEU:HD23	1:A:147:LEU:C	2.38	0.48
1:C:152:TRP:CD1	1:C:161:VAL:HG21	2.49	0.48
1:D:106:TRP:HB3	1:D:130:CYS:HB3	1.95	0.48
1:A:27:GLY:O	1:A:28:THR:C	2.57	0.48
1:C:47:GLU:HB2	1:C:52:PHE:CE1	2.49	0.48
1:B:368:ASN:OD1	1:B:370:LYS:HD2	2.14	0.48
1:C:316:VAL:O	1:C:320:ASN:HB2	2.13	0.48
1:D:93:ILE:HG23	1:D:99:TYR:OH	2.14	0.48
1:D:259:ARG:HG3	1:D:259:ARG:HH11	1.79	0.48
1:A:15:LEU:O	1:A:16:PRO:C	2.57	0.48
1:D:386:VAL:HG12	1:D:387:LEU:N	2.29	0.48
1:A:72:ASP:HB2	1:A:78:LEU:CD2	2.44	0.47
1:A:171:LEU:HA	1:A:174:ARG:NH1	2.29	0.47
1:B:283:CYS:SG	1:B:307:MET:HG3	2.54	0.47
1:D:69:THR:HA	1:D:78:LEU:O	2.14	0.47
1:C:111:MET:HB2	1:C:125:PHE:CZ	2.49	0.47
1:D:136:GLN:O	1:D:287:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:TRP:HA	1:D:379:TRP:CE3	2.47	0.47
1:A:45:ILE:HD13	1:A:81:ARG:CZ	2.44	0.47
1:B:21:ILE:H	1:B:21:ILE:CD1	2.26	0.47
1:D:263:TYR:CD2	1:D:291:LEU:HD13	2.46	0.47
1:A:116:ARG:O	1:A:118:GLN:HG3	2.15	0.47
1:C:256:ARG:HD2	1:C:256:ARG:C	2.39	0.47
1:C:364:HIS:HD2	1:D:104:ARG:HH22	1.58	0.47
1:D:51:LEU:HD21	1:D:295:LEU:HD13	1.96	0.47
1:A:111:MET:HB2	1:A:125:PHE:CZ	2.49	0.47
1:C:234:ARG:HA	1:C:234:ARG:HD3	1.74	0.47
1:D:73:ARG:CG	1:D:73:ARG:NH1	2.78	0.47
1:D:259:ARG:HG2	1:D:268:VAL:CG1	2.45	0.47
1:D:367:GLY:HA2	1:D:371:LYS:HD2	1.95	0.47
1:A:32:VAL:CG1	1:A:150:ARG:HD2	2.36	0.47
1:A:411:ALA:O	1:A:415:VAL:HG13	2.14	0.47
1:A:414:SER:O	1:A:418:HIS:CD2	2.60	0.47
1:B:148:THR:HB	1:B:152:TRP:CZ2	2.49	0.47
1:C:334:VAL:HG21	1:C:373:PHE:HE1	1.75	0.47
1:D:383:VAL:CG2	1:D:422:LEU:HD13	2.44	0.47
1:A:333:LEU:HD23	1:A:334:VAL:O	2.15	0.47
1:B:231:GLU:O	1:B:235:GLU:HG3	2.15	0.47
1:B:242:LYS:O	1:B:243:LEU:C	2.56	0.47
1:B:367:GLY:HA2	1:B:371:LYS:HD2	1.96	0.47
1:C:44:PRO:O	1:C:81:ARG:NH1	2.48	0.47
1:C:179:ASP:O	1:C:183:ALA:HB2	2.15	0.47
1:D:51:LEU:HD22	1:D:86:ALA:HB1	1.97	0.47
1:D:67:MET:HE3	1:D:67:MET:HB3	1.67	0.47
1:B:89:VAL:HG11	1:B:291:LEU:CD2	2.45	0.47
1:C:311:ARG:NH2	3:C:452:ATP:N3	2.62	0.47
1:C:369:PHE:HA	1:C:372:GLN:HG3	1.97	0.47
1:D:410:VAL:HG12	1:D:411:ALA:N	2.29	0.47
1:B:241:CYS:HB2	1:B:242:LYS:HE2	1.97	0.47
1:A:184:PHE:CD1	1:A:184:PHE:C	2.93	0.46
1:B:112:PHE:N	1:B:112:PHE:CD1	2.82	0.46
1:D:72:ASP:HB2	1:D:78:LEU:HD21	1.97	0.46
1:A:171:LEU:O	1:A:175:ALA:N	2.47	0.46
1:C:46:VAL:HG22	1:D:11:MET:SD	2.55	0.46
1:C:60:THR:O	1:C:64:GLU:HG3	2.15	0.46
1:A:272:VAL:HG12	1:A:281:THR:HA	1.96	0.46
1:B:8:ILE:O	1:B:9:ARG:C	2.58	0.46
1:C:36:TYR:HB3	1:C:38:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ASP:HA	1:C:243:LEU:CD1	2.45	0.46
1:C:385:VAL:HG12	1:C:385:VAL:O	2.15	0.46
1:D:81:ARG:HA	1:D:82:PRO:HD2	1.75	0.46
1:A:351:LEU:HD21	1:A:415:VAL:CG2	2.45	0.46
1:B:67:MET:HE3	1:B:67:MET:HB3	1.68	0.46
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.75	0.46
1:D:135:LEU:HD13	1:D:140:ILE:HG12	1.97	0.46
1:A:46:VAL:HG23	1:B:8:ILE:HD12	1.98	0.46
1:A:47:GLU:OE2	1:A:90:ARG:HD3	2.15	0.46
1:B:113:ARG:O	1:B:123:ARG:HA	2.15	0.46
1:B:341:GLN:NE2	1:B:364:HIS:ND1	2.64	0.46
1:C:169:GLY:CA	1:C:229:LEU:HD21	2.43	0.46
1:D:33:LEU:HD13	1:D:106:TRP:CG	2.51	0.46
1:D:235:GLU:CG	1:D:236:HIS:N	2.79	0.46
1:B:121:ARG:NH1	3:B:452:ATP:O2G	2.48	0.46
1:C:345:MET:SD	1:C:364:HIS:CE1	3.09	0.46
1:D:291:LEU:HD21	1:D:295:LEU:HD11	1.98	0.46
1:B:121:ARG:NH1	3:B:452:ATP:O1G	2.45	0.46
1:B:157:ILE:HG22	1:B:319:VAL:CG1	2.46	0.46
1:D:122:TYR:H	3:D:452:ATP:HN62	1.64	0.46
1:A:22:TRP:CH2	1:A:310:GLU:HG3	2.49	0.46
1:B:89:VAL:HG11	1:B:291:LEU:HD23	1.97	0.46
1:B:138:PRO:HB3	1:B:240:LEU:HB2	1.96	0.46
1:B:160:HIS:ND1	1:B:319:VAL:HG21	2.31	0.46
1:B:287:ARG:NH2	1:B:303:VAL:HG21	2.31	0.46
1:B:312:LEU:HD23	1:B:312:LEU:C	2.41	0.46
1:B:368:ASN:CG	1:B:370:LYS:HD2	2.41	0.46
1:C:85:THR:OG1	2:C:451:HSO:CD2	2.64	0.46
1:D:152:TRP:HB3	1:D:157:ILE:HD12	1.98	0.46
1:A:8:ILE:O	1:A:9:ARG:C	2.58	0.46
1:A:150:ARG:HG3	1:A:150:ARG:HH11	1.81	0.46
1:A:382:ARG:HH21	1:A:423:LEU:HD22	1.81	0.46
1:B:25:ILE:HG21	1:B:312:LEU:HD21	1.98	0.46
1:C:332:TYR:OH	1:C:363:ASN:HB2	2.16	0.46
1:C:397:ALA:HB2	1:C:412:GLN:HE21	1.80	0.46
1:A:99:TYR:O	1:A:101:GLN:HG3	2.15	0.45
1:A:135:LEU:CD1	1:A:140:ILE:HG12	2.46	0.45
1:A:391:GLU:HA	1:A:396:THR:OG1	2.16	0.45
1:B:54:ARG:O	1:B:294:GLN:NE2	2.49	0.45
1:B:67:MET:HB3	1:B:79:THR:HG21	1.98	0.45
1:A:287:ARG:NH1	1:A:303:VAL:HG21	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG12	1:A:80:LEU:HA	1.99	0.45
1:C:110:PRO:C	1:C:111:MET:HE2	2.41	0.45
1:D:343:ALA:O	1:D:346:ALA:HB3	2.17	0.45
1:A:165:LEU:CD1	1:A:269:PHE:HB3	2.47	0.45
1:B:157:ILE:HD13	1:B:315:LEU:HD23	1.99	0.45
1:A:48:GLN:HB3	1:A:50:PRO:HD2	1.97	0.45
1:A:59:VAL:HG22	1:A:59:VAL:O	2.17	0.45
1:A:259:ARG:CG	1:A:259:ARG:NH1	2.77	0.45
1:B:288:TYR:CE1	1:B:302:ALA:CB	2.99	0.45
1:A:261:LEU:N	1:A:261:LEU:HD22	2.31	0.45
1:A:412:GLN:HA	1:A:415:VAL:HG13	1.99	0.45
1:C:17:GLY:O	1:C:21:ILE:HD12	2.17	0.45
1:D:259:ARG:HB2	1:D:264:TYR:HD2	1.80	0.45
1:D:361:MET:HE1	1:D:379:TRP:NE1	2.31	0.45
1:A:5:ILE:CG2	1:A:6:GLN:N	2.79	0.45
1:A:60:THR:HG22	1:A:62:VAL:HG23	1.99	0.45
1:B:89:VAL:O	1:B:93:ILE:HG13	2.17	0.45
1:D:127:GLN:HE22	3:D:452:ATP:H5'1	1.81	0.45
1:D:152:TRP:CE3	1:D:157:ILE:HD11	2.52	0.45
1:D:160:HIS:O	1:D:161:VAL:HG13	2.16	0.45
1:B:14:TYR:HE2	1:B:126:HIS:CE1	2.32	0.45
1:B:331:ILE:HD13	1:B:358:VAL:CG1	2.47	0.45
1:C:32:VAL:HG13	1:C:150:ARG:CD	2.47	0.45
1:C:45:ILE:HG12	1:D:124:GLN:OE1	2.17	0.45
1:C:334:VAL:HG12	1:C:369:PHE:HE1	1.81	0.45
1:C:368:ASN:ND2	1:C:371:LYS:HB2	2.32	0.45
1:A:151:TRP:O	1:A:155:LEU:HD22	2.17	0.45
1:B:369:PHE:H	1:B:370:LYS:HZ2	1.65	0.45
1:B:419:LEU:HA	1:B:419:LEU:HD23	1.67	0.45
1:C:4:ASN:HD21	1:D:93:ILE:HG21	1.82	0.45
1:D:241:CYS:SG	1:D:251:TYR:OH	2.54	0.45
1:A:254:ASN:HD21	1:A:256:ARG:CZ	2.29	0.44
1:C:305:PHE:CD1	1:C:305:PHE:C	2.96	0.44
1:D:25:ILE:HD12	1:D:313:VAL:HG22	1.99	0.44
1:A:57:GLY:O	1:A:63:VAL:HG21	2.16	0.44
1:A:127:GLN:NE2	3:A:452:ATP:H5'1	2.32	0.44
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.66	0.44
1:B:125:PHE:CD2	3:B:452:ATP:C6	3.05	0.44
1:B:341:GLN:NE2	1:B:364:HIS:HA	2.33	0.44
1:B:350:ARG:NH1	1:B:412:GLN:HB3	2.31	0.44
1:C:163:LEU:HD12	1:C:165:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ASP:C	1:D:74:ASN:N	2.75	0.44
1:A:49:THR:HG23	1:A:79:THR:OG1	2.17	0.44
1:B:20:ALA:HB3	1:B:21:ILE:HD12	1.99	0.44
1:B:244:LEU:HD13	1:B:244:LEU:HA	1.84	0.44
1:C:112:PHE:HZ	1:D:45:ILE:HG13	1.83	0.44
1:B:15:LEU:HD22	1:B:15:LEU:H	1.82	0.44
1:C:116:ARG:HG3	1:C:116:ARG:NH1	2.28	0.44
1:D:98:LEU:CD2	1:D:133:PHE:HD2	2.30	0.44
1:D:290:GLY:O	1:D:293:GLU:HG2	2.17	0.44
1:A:274:ASN:N	1:A:274:ASN:HD22	2.15	0.44
1:C:174:ARG:HA	1:C:177:TYR:HB3	1.99	0.44
1:D:163:LEU:HD23	1:D:251:TYR:HB3	1.98	0.44
1:A:97:LEU:N	1:A:97:LEU:CD2	2.81	0.44
1:B:291:LEU:O	1:B:295:LEU:HG	2.18	0.44
1:B:320:ASN:C	1:B:322:GLU:N	2.75	0.44
1:D:148:THR:HG22	1:D:152:TRP:CZ2	2.53	0.44
1:D:234:ARG:CG	1:D:234:ARG:NH1	2.77	0.44
1:D:369:PHE:HB3	1:D:373:PHE:HE2	1.83	0.44
1:B:73:ARG:HG3	4:B:512:HOH:O	2.18	0.44
1:C:40:GLU:HG2	1:D:19:THR:HB	2.00	0.44
1:C:45:ILE:O	1:C:81:ARG:HG2	2.18	0.44
1:C:386:VAL:HB	1:C:398:VAL:HB	1.99	0.44
1:D:253:VAL:O	1:D:253:VAL:HG13	2.18	0.44
1:D:332:TYR:HE2	1:D:361:MET:HE2	1.81	0.44
1:D:332:TYR:OH	1:D:363:ASN:OD1	2.33	0.44
1:B:49:THR:O	1:B:50:PRO:C	2.61	0.44
1:C:15:LEU:O	1:C:16:PRO:C	2.61	0.44
1:C:52:PHE:CD2	1:C:82:PRO:HD2	2.52	0.44
1:C:326:ASP:HB2	1:C:359:LYS:NZ	2.33	0.44
1:A:16:PRO:HG3	1:B:105:LEU:CD2	2.48	0.43
1:A:88:CYS:O	1:A:89:VAL:C	2.60	0.43
1:B:148:THR:O	1:B:151:TRP:HB2	2.18	0.43
1:B:159:GLU:H	1:B:159:GLU:CD	2.25	0.43
1:C:5:ILE:HD12	1:D:51:LEU:CG	2.45	0.43
1:C:12:ASN:H	1:C:12:ASN:HD22	1.62	0.43
1:C:38:TYR:CD2	1:C:104:ARG:HB3	2.53	0.43
1:C:166:ASN:O	1:C:268:VAL:HG22	2.18	0.43
1:C:274:ASN:OD1	1:C:275:SER:N	2.50	0.43
1:A:233:SER:OG	1:A:266:ARG:HG2	2.19	0.43
1:B:330:ASP:C	1:B:331:ILE:HD12	2.43	0.43
1:D:288:TYR:O	1:D:288:TYR:CD1	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HD13	1:A:268:VAL:HG12	2.00	0.43
1:A:291:LEU:HD12	1:A:291:LEU:O	2.17	0.43
1:B:333:LEU:HB3	1:B:362:THR:HA	2.01	0.43
1:B:336:SER:O	1:B:340:THR:HG21	2.18	0.43
1:B:85:THR:O	1:B:89:VAL:CG2	2.66	0.43
1:C:43:LEU:HA	1:C:44:PRO:HD3	1.86	0.43
1:D:15:LEU:O	1:D:16:PRO:C	2.61	0.43
1:D:47:GLU:HB2	1:D:52:PHE:CZ	2.53	0.43
1:D:145:ILE:HG13	1:D:145:ILE:H	1.50	0.43
1:D:320:ASN:N	1:D:321:PRO:HD3	2.33	0.43
1:D:383:VAL:HG11	1:D:419:LEU:HD23	1.98	0.43
1:A:45:ILE:HG12	1:B:124:GLN:NE2	2.31	0.43
1:A:90:ARG:NH2	1:B:13:ASP:OD2	2.49	0.43
1:B:158:SER:C	1:B:160:HIS:H	2.27	0.43
1:B:288:TYR:O	1:B:288:TYR:HD1	2.01	0.43
1:B:391:GLU:OE1	1:B:391:GLU:N	2.51	0.43
1:C:251:TYR:HD1	1:C:251:TYR:H	1.66	0.43
1:C:331:ILE:N	1:C:331:ILE:HD12	2.33	0.43
1:D:49:THR:N	1:D:50:PRO:HD2	2.32	0.43
1:C:141:ASP:OD1	1:C:287:ARG:NH2	2.51	0.43
1:C:312:LEU:HA	1:C:312:LEU:HD12	1.77	0.43
1:A:167:SER:HB2	1:A:237:PHE:CD1	2.54	0.43
1:A:169:GLY:HA3	1:A:229:LEU:CD2	2.48	0.43
1:B:98:LEU:HD22	1:B:133:PHE:CD2	2.52	0.43
1:B:161:VAL:HG23	1:B:271:TRP:CE3	2.54	0.43
1:C:40:GLU:O	1:D:19:THR:HG21	2.19	0.43
1:D:329:VAL:HB	1:D:379:TRP:HB3	2.01	0.43
1:D:340:THR:O	1:D:343:ALA:N	2.51	0.43
1:D:383:VAL:CG1	1:D:384:ALA:N	2.81	0.43
1:A:386:VAL:HG12	1:A:387:LEU:N	2.34	0.43
1:B:29:LEU:HD13	1:B:307:MET:HE1	2.01	0.43
1:B:41:ILE:O	1:B:41:ILE:HG23	2.19	0.43
1:B:108:ILE:HB	1:B:128:LEU:HD12	1.99	0.43
1:B:314:LEU:HA	1:B:317:GLN:OE1	2.19	0.43
1:C:163:LEU:HD23	1:C:271:TRP:NE1	2.33	0.43
1:C:164:GLU:HA	1:C:252:THR:O	2.19	0.43
1:D:128:LEU:HB3	1:D:309:LEU:HD11	2.00	0.43
1:A:49:THR:N	1:A:50:PRO:CD	2.81	0.43
1:A:152:TRP:HB3	1:A:158:SER:HA	2.01	0.43
1:B:81:ARG:HA	1:B:82:PRO:HD2	1.98	0.43
1:C:19:THR:O	1:C:22:TRP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ASN:ND2	1:D:168:ILE:HD13	2.34	0.43
1:D:287:ARG:O	1:D:288:TYR:HB3	2.19	0.43
1:D:292:VAL:HG21	1:D:300:THR:HG22	2.01	0.43
1:D:324:LYS:HD2	1:D:324:LYS:N	2.34	0.43
1:D:386:VAL:HB	1:D:398:VAL:HB	2.01	0.43
1:A:91:ALA:HA	1:A:94:GLU:HB3	2.01	0.42
1:A:363:ASN:CG	1:A:364:HIS:N	2.77	0.42
1:B:30:LYS:O	1:B:33:LEU:HB2	2.19	0.42
1:D:314:LEU:HD23	1:D:314:LEU:HA	1.82	0.42
1:C:47:GLU:HB2	1:C:52:PHE:HE1	1.84	0.42
1:C:331:ILE:HD12	1:C:331:ILE:H	1.84	0.42
1:A:278:SER:CA	1:A:311:ARG:HD3	2.49	0.42
1:A:319:VAL:HG12	1:A:320:ASN:HD22	1.82	0.42
1:B:5:ILE:N	1:B:5:ILE:HD12	2.33	0.42
1:B:83:GLU:OE2	1:B:85:THR:HB	2.19	0.42
1:B:232:GLU:OE1	1:B:266:ARG:NH1	2.51	0.42
1:B:370:LYS:H	1:B:370:LYS:CE	2.31	0.42
1:C:146:MET:HE1	1:D:345:MET:SD	2.59	0.42
1:C:181:LEU:O	1:C:184:PHE:HB3	2.19	0.42
1:C:334:VAL:CG1	1:C:373:PHE:HE1	2.26	0.42
1:D:8:ILE:O	1:D:9:ARG:C	2.62	0.42
1:D:40:GLU:HG3	1:D:106:TRP:CH2	2.55	0.42
1:D:168:ILE:O	1:D:168:ILE:HG23	2.20	0.42
1:D:323:PHE:CD1	1:D:323:PHE:C	2.97	0.42
1:B:15:LEU:O	1:B:16:PRO:C	2.62	0.42
1:C:347:LEU:HG	1:C:351:LEU:HD11	2.00	0.42
1:D:147:LEU:HD23	1:D:147:LEU:C	2.44	0.42
1:D:68:TYR:OH	1:D:123:ARG:NE	2.52	0.42
1:A:139:ASP:HA	1:A:243:LEU:HD23	2.01	0.42
1:B:72:ASP:HB2	1:B:78:LEU:CD1	2.48	0.42
1:B:288:TYR:CE1	1:B:302:ALA:HB1	2.55	0.42
1:C:63:VAL:HA	1:C:67:MET:SD	2.60	0.42
1:A:165:LEU:HD13	1:A:269:PHE:CB	2.49	0.42
1:A:166:ASN:O	1:A:268:VAL:N	2.50	0.42
1:D:46:VAL:CG1	1:D:80:LEU:HD12	2.35	0.42
1:A:34:GLY:C	1:A:36:TYR:N	2.78	0.42
1:B:157:ILE:HG22	1:B:319:VAL:HG11	2.01	0.42
1:B:259:ARG:HB2	1:B:264:TYR:CD2	2.55	0.42
1:C:291:LEU:HD23	1:C:291:LEU:C	2.45	0.42
1:C:347:LEU:HD12	1:C:347:LEU:HA	1.80	0.42
1:D:125:PHE:CE1	1:D:127:GLN:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:MET:CE	1:B:379:TRP:NE1	2.83	0.42
1:C:163:LEU:CD1	1:C:165:LEU:HD12	2.50	0.42
1:D:46:VAL:HG12	1:D:79:THR:C	2.44	0.42
1:D:259:ARG:CG	1:D:268:VAL:HG13	2.48	0.42
1:A:10:GLY:O	1:A:123:ARG:N	2.51	0.42
1:A:111:MET:HE3	1:A:127:GLN:OE1	2.19	0.42
1:A:287:ARG:NH1	1:A:303:VAL:HG22	2.35	0.42
1:C:45:ILE:CD1	1:C:81:ARG:NH2	2.83	0.42
1:D:235:GLU:HG2	1:D:236:HIS:H	1.81	0.42
1:A:34:GLY:O	1:A:36:TYR:N	2.52	0.41
1:A:80:LEU:HD23	1:A:112:PHE:CD2	2.55	0.41
1:A:112:PHE:CD1	1:A:112:PHE:N	2.88	0.41
1:C:307:MET:SD	1:C:312:LEU:HD22	2.60	0.41
1:A:410:VAL:HG12	1:A:411:ALA:O	2.20	0.41
1:B:161:VAL:HA	1:B:272:VAL:O	2.20	0.41
1:C:334:VAL:HG21	1:C:373:PHE:CD1	2.53	0.41
1:D:157:ILE:HD12	1:D:157:ILE:C	2.46	0.41
1:A:231:GLU:OE1	1:A:231:GLU:HA	2.21	0.41
1:A:383:VAL:HG11	1:A:422:LEU:CD1	2.49	0.41
1:C:34:GLY:C	1:C:36:TYR:N	2.77	0.41
1:A:44:PRO:HA	1:B:124:GLN:OE1	2.19	0.41
1:A:68:TYR:HB2	1:A:80:LEU:HB2	2.03	0.41
1:B:139:ASP:HA	1:B:243:LEU:HD13	2.02	0.41
1:C:81:ARG:HE	1:C:111:MET:HE2	1.85	0.41
1:B:33:LEU:HD11	1:B:128:LEU:HD21	2.00	0.41
1:B:52:PHE:HB2	1:B:67:MET:HE1	2.03	0.41
1:D:391:GLU:HG2	1:D:398:VAL:HG23	2.02	0.41
1:D:394:ASN:O	1:D:396:THR:HG23	2.20	0.41
1:A:105:LEU:O	1:A:130:CYS:HB2	2.20	0.41
1:A:230:ASP:OD2	1:A:233:SER:HB2	2.21	0.41
1:B:9:ARG:HE	1:B:116:ARG:NH2	2.15	0.41
1:D:257:LEU:HD21	1:D:270:GLU:HG2	2.03	0.41
1:A:90:ARG:NH2	1:B:7:ALA:HB2	2.36	0.41
1:B:102:GLU:OE2	1:B:135:LEU:HD21	2.20	0.41
1:D:89:VAL:HG21	1:D:291:LEU:HD22	2.03	0.41
1:D:265:ASN:HD22	1:D:288:TYR:HA	1.85	0.41
1:D:283:CYS:SG	1:D:307:MET:HB2	2.60	0.41
1:A:34:GLY:C	1:A:36:TYR:H	2.29	0.41
1:A:175:ALA:C	1:A:177:TYR:H	2.28	0.41
1:A:383:VAL:CG2	1:A:422:LEU:HD22	2.51	0.41
1:B:244:LEU:HD12	1:B:249:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ASN:HD22	1:B:266:ARG:NE	2.15	0.41
1:C:106:TRP:HB3	1:C:130:CYS:HB3	2.03	0.41
1:D:103:GLN:OE1	1:D:103:GLN:HA	2.21	0.41
1:B:287:ARG:HG3	1:B:302:ALA:O	2.21	0.41
1:C:105:LEU:HD23	1:C:105:LEU:H	1.84	0.41
1:C:147:LEU:C	1:C:147:LEU:CD2	2.92	0.41
1:C:363:ASN:CG	1:C:364:HIS:N	2.79	0.41
1:D:322:GLU:HA	1:D:324:LYS:NZ	2.36	0.41
1:D:415:VAL:HG12	1:D:419:LEU:CD1	2.51	0.41
1:A:410:VAL:CG1	1:A:411:ALA:N	2.84	0.41
1:B:130:CYS:SG	1:B:305:PHE:HE1	2.44	0.41
1:C:44:PRO:HA	1:D:124:GLN:NE2	2.32	0.41
1:C:102:GLU:OE1	1:C:135:LEU:HD21	2.21	0.41
1:C:171:LEU:N	1:C:171:LEU:HD13	2.36	0.41
1:A:4:ASN:N	1:B:54:ARG:HH22	2.18	0.40
1:B:91:ALA:O	1:B:95:HIS:CD2	2.68	0.40
1:B:138:PRO:O	1:B:139:ASP:C	2.64	0.40
1:B:235:GLU:HG3	1:B:235:GLU:H	1.75	0.40
1:B:341:GLN:HE22	1:B:364:HIS:HA	1.84	0.40
1:C:56:ILE:HG23	1:C:261:LEU:HD13	2.03	0.40
1:C:329:VAL:CG2	1:C:361:MET:HE3	2.51	0.40
1:D:128:LEU:CB	1:D:309:LEU:HD11	2.51	0.40
1:D:263:TYR:HB3	1:D:291:LEU:CD1	2.51	0.40
1:D:259:ARG:NH1	1:D:264:TYR:CZ	2.89	0.40
1:B:397:ALA:HB3	1:B:415:VAL:HG21	2.03	0.40
1:C:5:ILE:HG21	1:D:48:GLN:HB2	2.04	0.40
1:C:73:ARG:HA	1:C:73:ARG:HD3	1.65	0.40
1:C:174:ARG:O	1:C:177:TYR:N	2.54	0.40
1:C:254:ASN:HD21	1:C:256:ARG:CZ	2.35	0.40
1:C:275:SER:O	1:C:276:LEU:C	2.64	0.40
1:D:273:THR:CG2	1:D:277:GLY:H	2.35	0.40
1:D:311:ARG:HD3	3:D:452:ATP:C2	2.56	0.40
1:D:368:ASN:HD21	1:D:371:LYS:HE3	1.84	0.40
1:D:355:LEU:HB3	1:D:358:VAL:HG21	2.03	0.40
1:A:41:ILE:O	1:A:41:ILE:HG23	2.21	0.40
1:A:121:ARG:H	1:A:121:ARG:HG2	1.59	0.40
1:A:273:THR:C	1:A:275:SER:N	2.79	0.40
1:B:47:GLU:OE2	1:B:90:ARG:HD3	2.21	0.40
1:B:163:LEU:HD23	1:B:251:TYR:HB3	2.03	0.40
1:B:374:ALA:O	1:B:377:ASP:HB2	2.21	0.40
1:C:56:ILE:HG12	1:C:261:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:PHE:CE1	1:D:302:ALA:HB1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	375/424 (88%)	326 (87%)	38 (10%)	11 (3%)	3	13
1	B	360/424 (85%)	317 (88%)	35 (10%)	8 (2%)	5	19
1	C	383/424 (90%)	331 (86%)	41 (11%)	11 (3%)	3	13
1	D	360/424 (85%)	317 (88%)	38 (11%)	5 (1%)	9	30
All	All	1478/1696 (87%)	1291 (87%)	152 (10%)	35 (2%)	4	17

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	TYR
1	A	338	ALA
1	B	64	GLU
1	B	288	TYR
1	B	338	ALA
1	C	137	GLY
1	C	276	LEU
1	C	278	SER
1	C	288	TYR
1	C	338	ALA
1	D	288	TYR
1	A	8	ILE
1	A	73	ARG
1	A	137	GLY

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Mol	Chain	Res	Type
1	A	321	PRO
1	B	117	PRO
1	B	137	GLY
1	C	136	GLN
1	C	341	GLN
1	C	366	GLY
1	D	137	GLY
1	D	338	ALA
1	A	341	GLN
1	A	366	GLY
1	B	276	LEU
1	D	64	GLU
1	D	341	GLN
1	A	16	PRO
1	B	321	PRO
1	C	16	PRO
1	C	340	THR
1	B	341	GLN
1	A	82	PRO
1	A	365	GLY
1	C	365	GLY

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	299/342 (87%)	243 (81%)	56 (19%)	1	5
1	B	286/342 (84%)	229 (80%)	57 (20%)	1	5
1	C	301/342 (88%)	238 (79%)	63 (21%)	1	4
1	D	285/342 (83%)	226 (79%)	59 (21%)	1	4
All	All	1171/1368 (86%)	936 (80%)	235 (20%)	1	4

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	9	ARG
1	A	15	LEU
1	A	16	PRO
1	A	18	GLU
1	A	19	THR
1	A	21	ILE
1	A	23	GLN
1	A	35	SER
1	A	39	SER
1	A	48	GLN
1	A	65	LYS
1	A	78	LEU
1	A	97	LEU
1	A	105	LEU
1	A	116	ARG
1	A	121	ARG
1	A	128	LEU
1	A	132	VAL
1	A	139	ASP
1	A	140	ILE
1	A	141	ASP
1	A	155	LEU
1	A	161	VAL
1	A	165	LEU
1	A	174	ARG
1	A	232	GLU
1	A	235	GLU
1	A	243	LEU
1	A	246	SER
1	A	251	TYR
1	A	252	THR
1	A	255	GLN
1	A	256	ARG
1	A	257	LEU
1	A	259	ARG
1	A	261	LEU
1	A	263	TYR
1	A	276	LEU
1	A	281	THR
1	A	295	LEU
1	A	307	MET
1	A	324	LYS

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Mol	Chain	Res	Type
1	A	327	PRO
1	A	328	VAL
1	A	331	ILE
1	A	339	ASP
1	A	342	SER
1	A	354	GLU
1	A	362	THR
1	A	371	LYS
1	A	372	GLN
1	A	383	VAL
1	A	399	VAL
1	A	414	SER
1	A	421	THR
1	B	12	ASN
1	B	16	PRO
1	B	21	ILE
1	B	24	ARG
1	B	30	LYS
1	B	42	ARG
1	B	46	VAL
1	B	48	GLN
1	B	54	ARG
1	B	58	GLU
1	B	59	VAL
1	B	67	MET
1	B	71	GLU
1	B	77	SER
1	B	79	THR
1	B	89	VAL
1	B	90	ARG
1	B	105	LEU
1	B	108	ILE
1	B	116	ARG
1	B	118	GLN
1	B	128	LEU
1	B	131	GLU
1	B	132	VAL
1	B	135	LEU
1	B	139	ASP
1	B	157	ILE
1	B	159	GLU
1	B	165	LEU

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Mol	Chain	Res	Type
1	B	235	GLU
1	B	251	TYR
1	B	252	THR
1	B	256	ARG
1	B	257	LEU
1	B	259	ARG
1	B	261	LEU
1	B	263	TYR
1	B	272	VAL
1	B	274	ASN
1	B	293	GLU
1	B	298	ARG
1	B	303	VAL
1	B	307	MET
1	B	322	GLU
1	B	331	ILE
1	B	333	LEU
1	B	339	ASP
1	B	340	THR
1	B	342	SER
1	B	345	MET
1	B	360	LEU
1	B	370	LYS
1	B	382	ARG
1	B	404	SER
1	B	407	GLN
1	B	408	THR
1	B	414	SER
1	C	5	ILE
1	C	12	ASN
1	C	16	PRO
1	C	24	ARG
1	C	35	SER
1	C	39	SER
1	C	40	GLU
1	C	48	GLN
1	C	62	VAL
1	C	73	ARG
1	C	74	ASN
1	C	78	LEU
1	C	80	LEU
1	C	83	GLU

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Mol	Chain	Res	Type
1	C	105	LEU
1	C	108	ILE
1	C	116	ARG
1	C	117	PRO
1	C	119	LYS
1	C	128	LEU
1	C	153	ARG
1	C	159	GLU
1	C	161	VAL
1	C	165	LEU
1	C	168	ILE
1	C	171	LEU
1	C	229	LEU
1	C	234	ARG
1	C	240	LEU
1	C	242	LYS
1	C	251	TYR
1	C	255	GLN
1	C	256	ARG
1	C	257	LEU
1	C	261	LEU
1	C	263	TYR
1	C	266	ARG
1	C	270	GLU
1	C	274	ASN
1	C	275	SER
1	C	276	LEU
1	C	287	ARG
1	C	303	VAL
1	C	320	ASN
1	C	322	GLU
1	C	324	LYS
1	C	327	PRO
1	C	331	ILE
1	C	339	ASP
1	C	342	SER
1	C	354	GLU
1	C	360	LEU
1	C	371	LYS
1	C	372	GLN
1	C	382	ARG
1	C	383	VAL

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Mol	Chain	Res	Type
1	C	387	LEU
1	C	389	GLU
1	C	400	LYS
1	C	406	GLU
1	C	412	GLN
1	C	421	THR
1	C	423	LEU
1	D	4	ASN
1	D	12	ASN
1	D	15	LEU
1	D	16	PRO
1	D	24	ARG
1	D	31	ASN
1	D	38	TYR
1	D	46	VAL
1	D	51	LEU
1	D	59	VAL
1	D	61	ASP
1	D	64	GLU
1	D	67	MET
1	D	78	LEU
1	D	100	ASN
1	D	101	GLN
1	D	103	GLN
1	D	105	LEU
1	D	115	GLU
1	D	118	GLN
1	D	121	ARG
1	D	126	HIS
1	D	131	GLU
1	D	132	VAL
1	D	140	ILE
1	D	145	ILE
1	D	148	THR
1	D	158	SER
1	D	161	VAL
1	D	168	ILE
1	D	231	GLU
1	D	232	GLU
1	D	234	ARG
1	D	240	LEU
1	D	245	GLU

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Mol	Chain	Res	Type
1	D	251	TYR
1	D	257	LEU
1	D	263	TYR
1	D	266	ARG
1	D	274	ASN
1	D	283	CYS
1	D	292	VAL
1	D	303	VAL
1	D	307	MET
1	D	309	LEU
1	D	311	ARG
1	D	319	VAL
1	D	320	ASN
1	D	328	VAL
1	D	333	LEU
1	D	341	GLN
1	D	342	SER
1	D	350	ARG
1	D	371	LYS
1	D	375	ARG
1	D	382	ARG
1	D	390	SER
1	D	401	ASP
1	D	421	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	31	ASN
1	A	95	HIS
1	A	101	GLN
1	A	236	HIS
1	A	255	GLN
1	A	274	ASN
1	A	317	GLN
1	A	320	ASN
1	A	363	ASN
1	A	372	GLN
1	A	418	HIS
1	B	12	ASN
1	B	95	HIS

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Mol	Chain	Res	Type
1	B	114	HIS
1	B	118	GLN
1	B	341	GLN
1	C	4	ASN
1	C	12	ASN
1	C	48	GLN
1	C	100	ASN
1	C	114	HIS
1	C	118	GLN
1	C	127	GLN
1	C	255	GLN
1	C	294	GLN
1	C	317	GLN
1	C	320	ASN
1	C	363	ASN
1	C	364	HIS
1	C	412	GLN
1	D	12	ASN
1	D	48	GLN
1	D	127	GLN
1	D	136	GLN
1	D	166	ASN
1	D	236	HIS
1	D	364	HIS
1	D	407	GLN
1	D	418	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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
3	ATP	A	452	-	32,33,33	0.73	1 (3%)	48,52,52	0.83	0
3	ATP	B	452	-	32,33,33	0.99	3 (9%)	48,52,52	0.77	1 (2%)
3	ATP	C	452	-	32,33,33	0.73	0	48,52,52	0.84	1 (2%)
2	HSO	D	451	-	10,10,10	1.35	1 (10%)	10,12,12	1.30	1 (10%)
2	HSO	C	451	-	10,10,10	1.37	1 (10%)	10,12,12	1.27	1 (10%)
2	HSO	A	451	-	10,10,10	1.44	1 (10%)	10,12,12	1.19	1 (10%)
3	ATP	D	452	-	32,33,33	0.62	0	48,52,52	0.81	2 (4%)
2	HSO	B	451	-	10,10,10	1.36	1 (10%)	10,12,12	1.31	1 (10%)

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
3	ATP	A	452	-	-	7/22/38/38	0/3/3/3
3	ATP	B	452	-	-	8/22/38/38	0/3/3/3
3	ATP	C	452	-	-	2/22/38/38	0/3/3/3
2	HSO	D	451	-	-	2/6/6/6	0/1/1/1
2	HSO	C	451	-	-	0/6/6/6	0/1/1/1
2	HSO	A	451	-	-	2/6/6/6	0/1/1/1
3	ATP	D	452	-	-	6/22/38/38	0/3/3/3
2	HSO	B	451	-	-	6/6/6/6	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	451	HSO	O-C	-4.46	1.23	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	451	HSO	O-C	-4.22	1.24	1.42
2	D	451	HSO	O-C	-4.17	1.24	1.42
2	B	451	HSO	O-C	-3.98	1.25	1.42
3	B	452	ATP	PA-O3A	3.14	1.62	1.59
3	B	452	ATP	PB-O3B	2.61	1.62	1.59
3	B	452	ATP	PB-O3A	2.53	1.62	1.59
3	A	452	ATP	PB-O3B	2.20	1.61	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	452	ATP	O3A-PB-O1B	-2.82	102.23	110.70
3	D	452	ATP	O3A-PB-O1B	-2.75	102.44	110.70
2	D	451	HSO	O-C-CA	2.55	121.33	111.52
2	C	451	HSO	O-C-CA	2.40	120.74	111.52
2	A	451	HSO	O-C-CA	2.30	120.36	111.52
3	B	452	ATP	O3A-PB-O1B	-2.27	103.87	110.70
2	B	451	HSO	O-C-CA	2.23	120.11	111.52
3	D	452	ATP	O3G-PG-O2G	2.00	115.31	107.80

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	451	HSO	O-C-CA-N
2	A	451	HSO	O-C-CA-CB
2	B	451	HSO	N-CA-CB-CG
2	B	451	HSO	C-CA-CB-CG
2	B	451	HSO	O-C-CA-CB
2	D	451	HSO	O-C-CA-CB
3	A	452	ATP	C5'-O5'-PA-O1A
3	A	452	ATP	C5'-O5'-PA-O3A
3	B	452	ATP	PB-O3A-PA-O5'
3	B	452	ATP	C5'-O5'-PA-O1A
3	B	452	ATP	C5'-O5'-PA-O2A
3	B	452	ATP	C5'-O5'-PA-O3A
3	D	452	ATP	C5'-O5'-PA-O1A
3	D	452	ATP	C5'-O5'-PA-O3A
3	C	452	ATP	PB-O3A-PA-O1A
3	D	452	ATP	PB-O3A-PA-O1A
2	B	451	HSO	O-C-CA-N
2	D	451	HSO	O-C-CA-N

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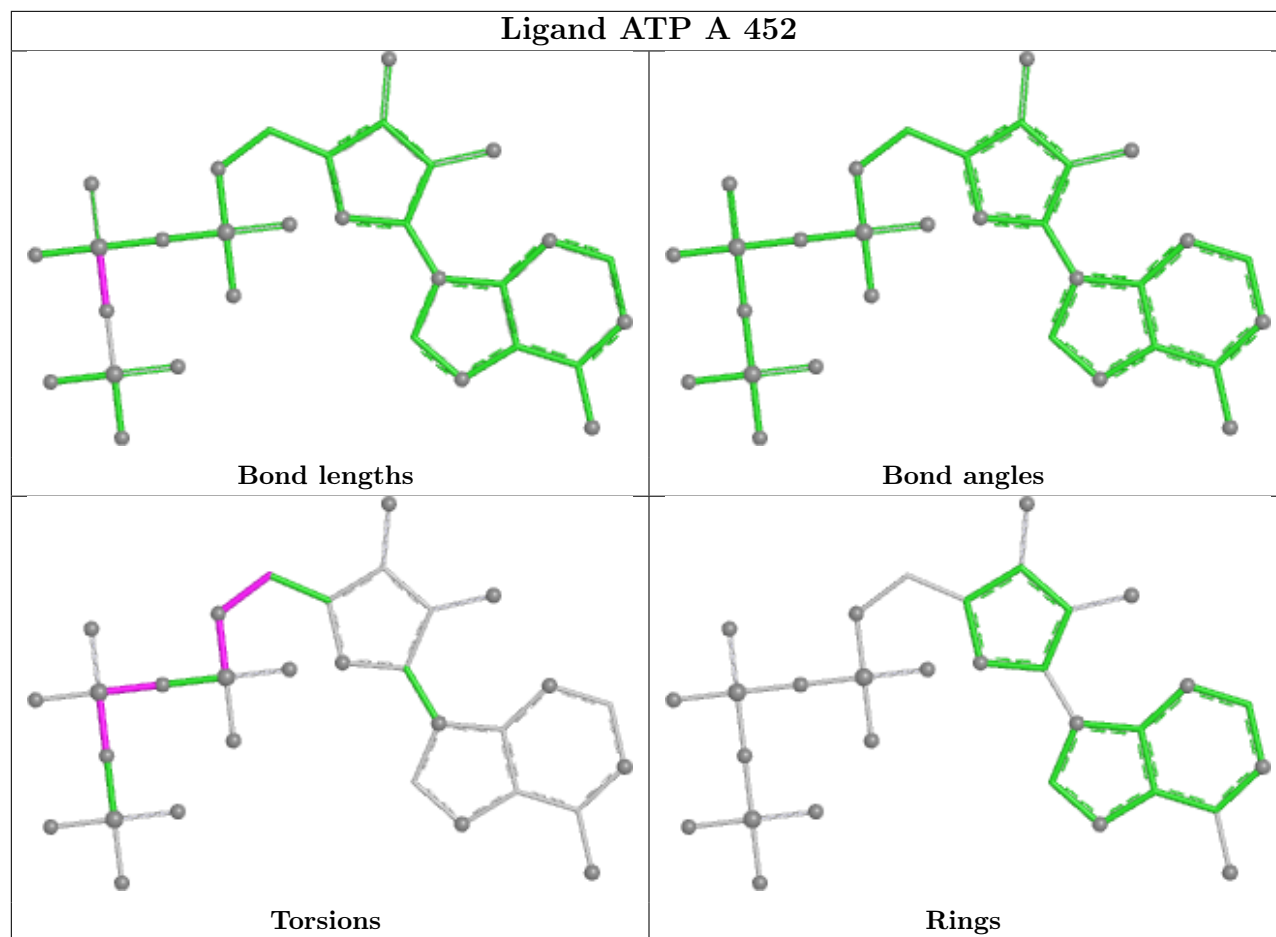
Mol	Chain	Res	Type	Atoms
3	A	452	ATP	C5'-O5'-PA-O2A
3	D	452	ATP	C5'-O5'-PA-O2A
3	D	452	ATP	PG-O3B-PB-O1B
3	D	452	ATP	PB-O3A-PA-O2A
3	A	452	ATP	C4'-C5'-O5'-PA
3	A	452	ATP	PG-O3B-PB-O2B
3	A	452	ATP	PG-O3B-PB-O1B
3	A	452	ATP	PA-O3A-PB-O2B
3	B	452	ATP	PA-O3A-PB-O2B
3	C	452	ATP	PB-O3A-PA-O2A
2	B	451	HSO	CA-CB-CG-CD2
2	B	451	HSO	CA-CB-CG-ND1
3	B	452	ATP	PG-O3B-PB-O1B
3	B	452	ATP	PG-O3B-PB-O2B
3	B	452	ATP	PA-O3A-PB-O1B

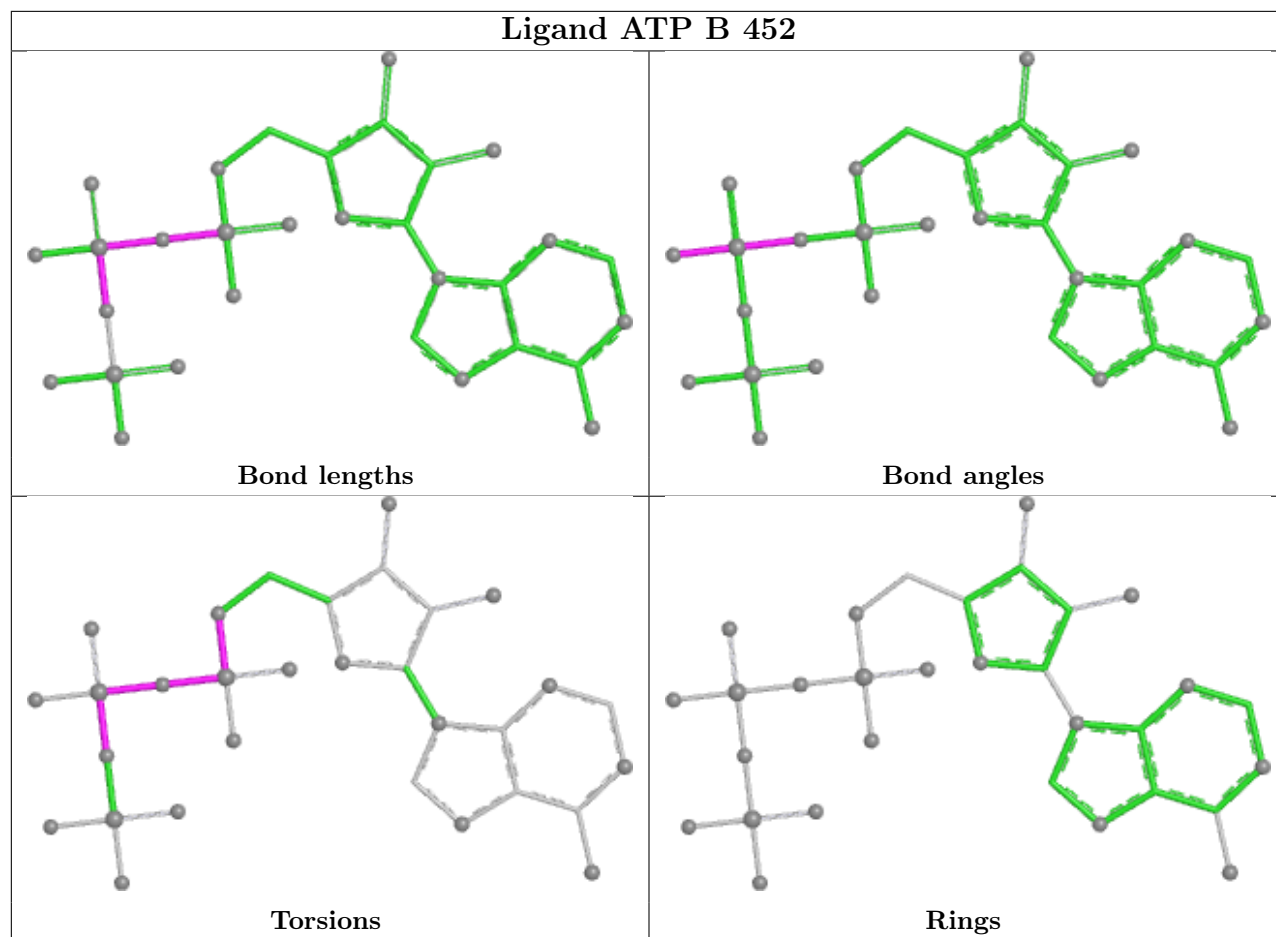
There are no ring outliers.

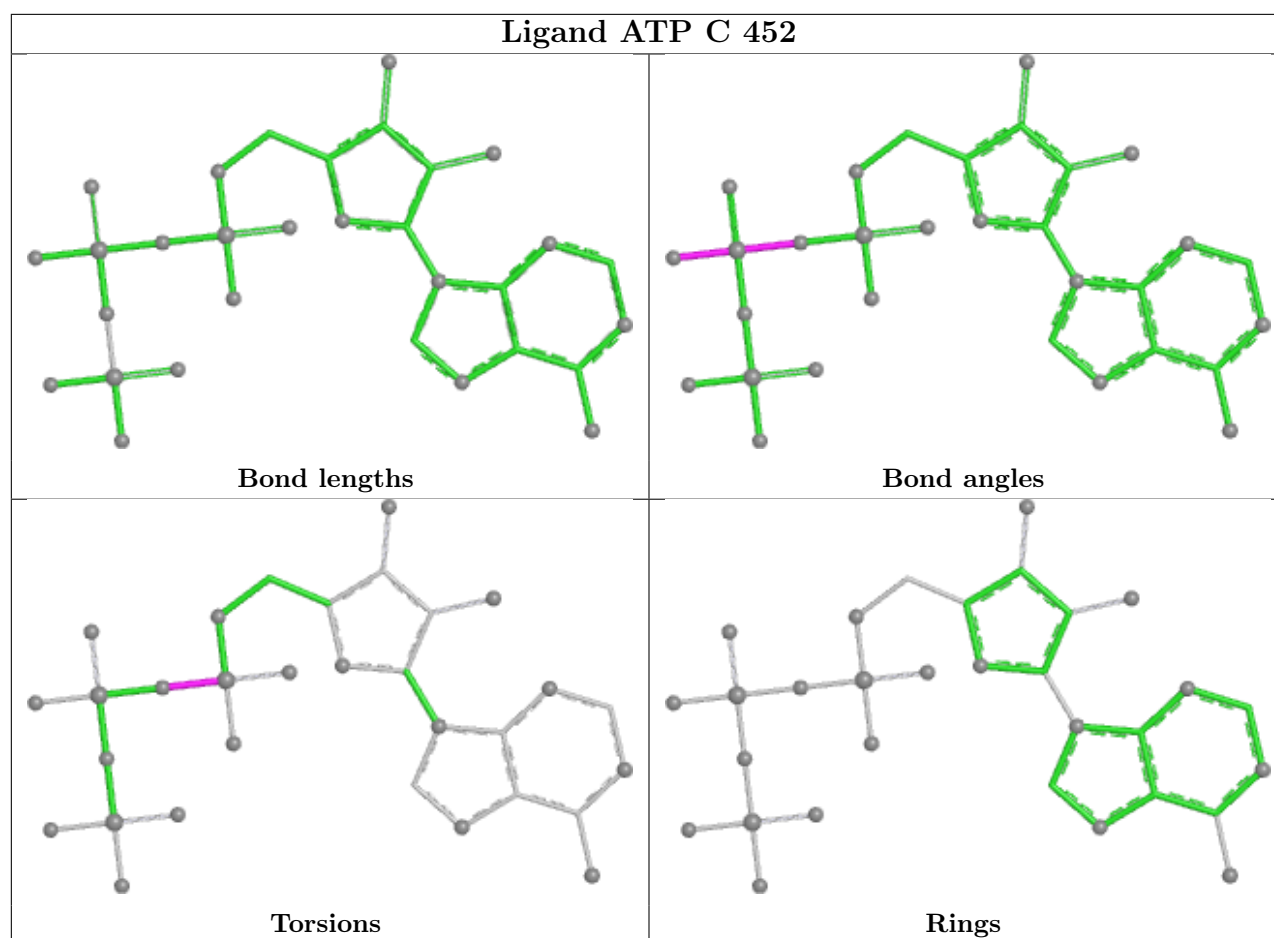
6 monomers are involved in 35 short contacts:

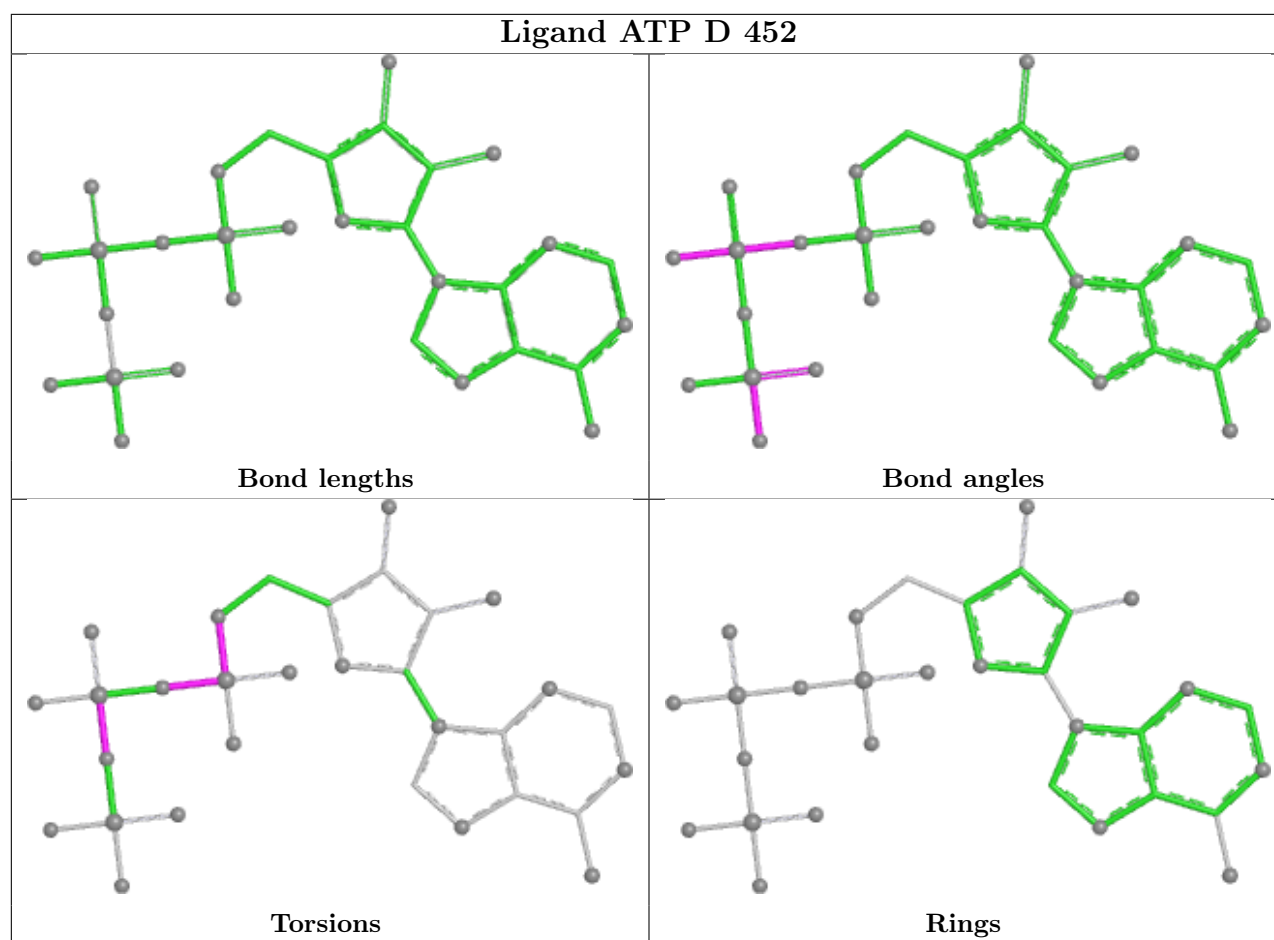
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	452	ATP	3	0
3	B	452	ATP	11	0
3	C	452	ATP	8	0
2	C	451	HSO	2	0
3	D	452	ATP	11	0
2	B	451	HSO	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	379/424 (89%)	-1.65	0 100 100	12, 34, 58, 73	0
1	B	364/424 (85%)	-1.63	0 100 100	14, 36, 62, 90	0
1	C	387/424 (91%)	-1.65	0 100 100	12, 34, 58, 72	0
1	D	364/424 (85%)	-1.63	0 100 100	14, 36, 63, 81	0
All	All	1494/1696 (88%)	-1.64	0 100 100	12, 35, 61, 90	0

There are no RSRZ outliers to report.

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.

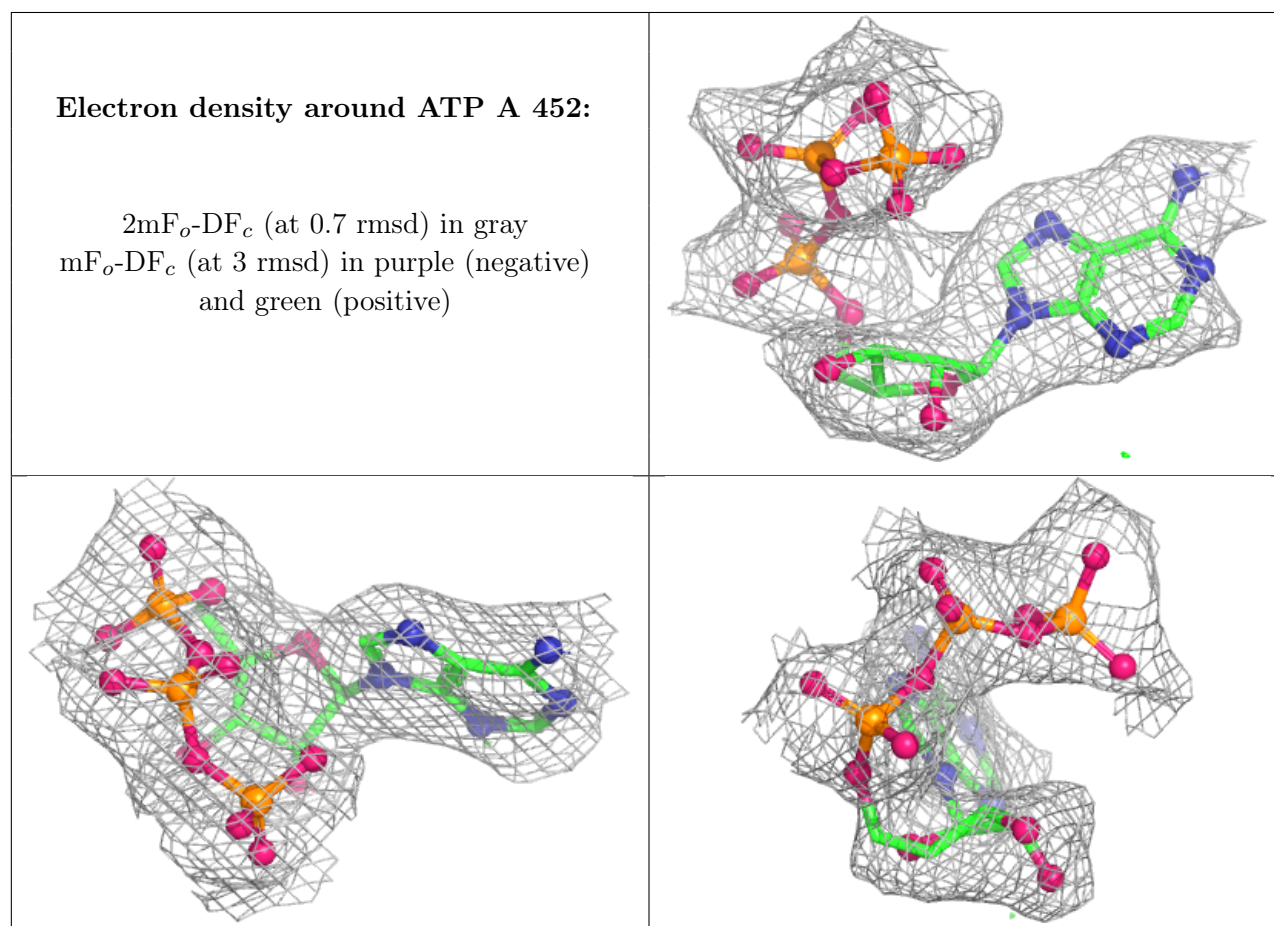
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HSO	B	451	10/10	0.99	0.04	0,26,32,32	0
2	HSO	C	451	10/10	0.99	0.04	0,31,35,41	0
2	HSO	D	451	10/10	0.99	0.03	0,35,38,40	0
3	ATP	A	452	31/31	0.99	0.03	0,35,47,52	0

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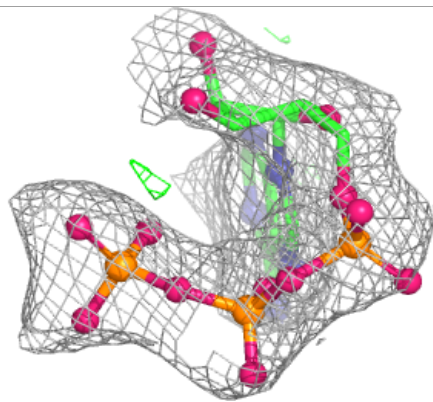
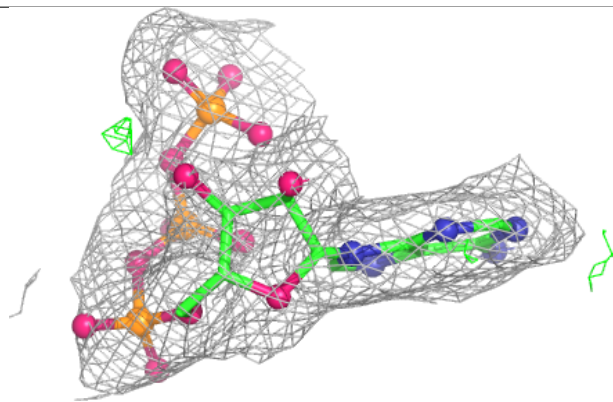
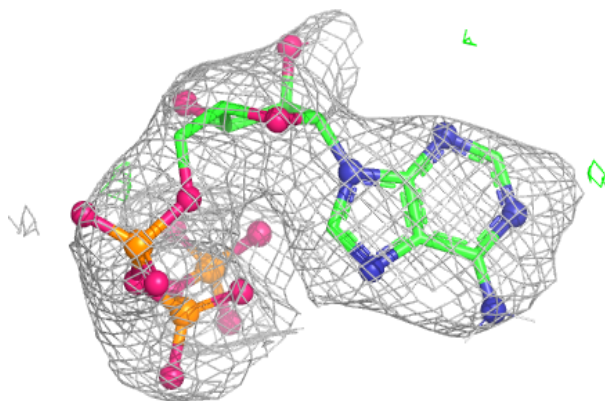
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	B	452	31/31	0.99	0.03	0,45,78,79	0
3	ATP	C	452	31/31	0.99	0.03	0,35,55,58	0
3	ATP	D	452	31/31	0.99	0.03	0,57,69,70	0
2	HSO	A	451	10/10	1.00	0.03	0,28,34,37	0

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.



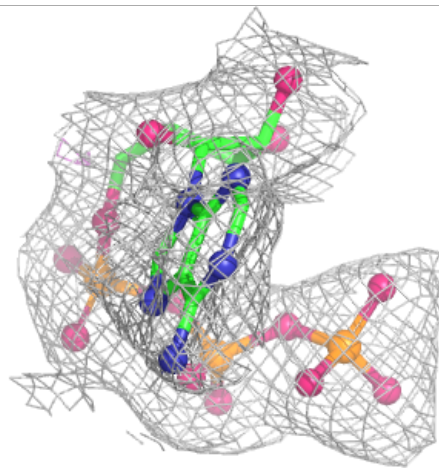
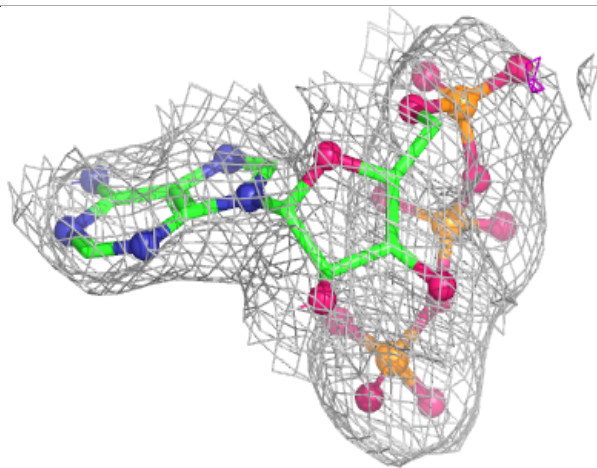
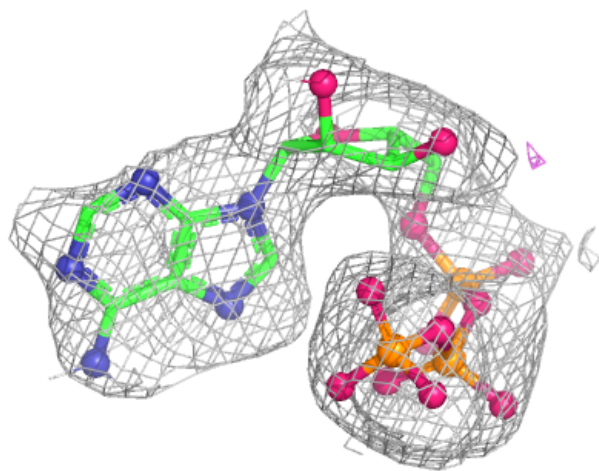
Electron density around ATP B 452:

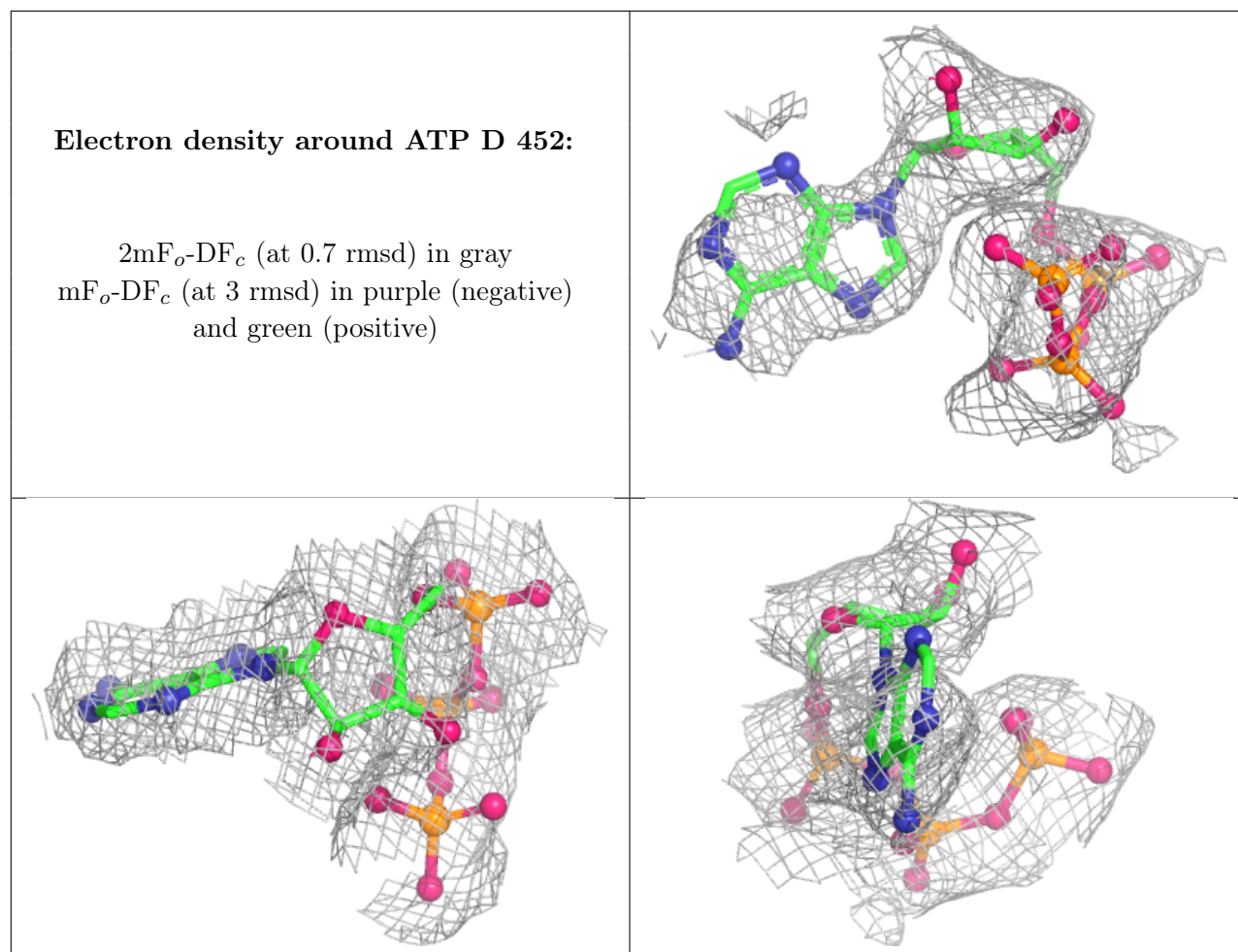
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP C 452:

$2mF_o-DF_c$ (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.