



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:26 PM UTC

PDB ID : 3O8L / pdb_00003o8l
Title : Structure of phosphofructokinase from rabbit skeletal muscle
Authors : Banaszak, K.; Chang, S.H.; Rypniewski, W.
Deposited on : 2010-08-03
Resolution : 3.20 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

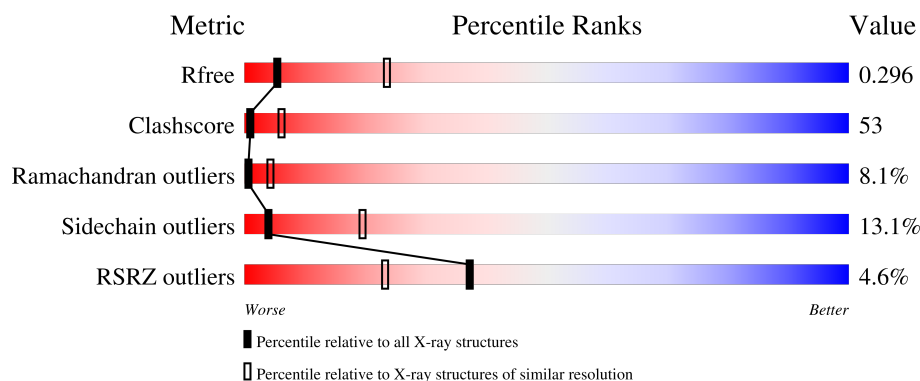
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	762	4% 31% 49% 16% ..
1	B	762	5% 32% 50% 15% ..

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
4	PO4	A	766	-	X	-	-
4	PO4	A	767	-	X	-	-
4	PO4	A	768	-	X	-	-
4	PO4	B	766	-	X	-	-
4	PO4	B	767	-	X	-	-
4	PO4	B	768	-	X	-	-

2 Entry composition [i](#)

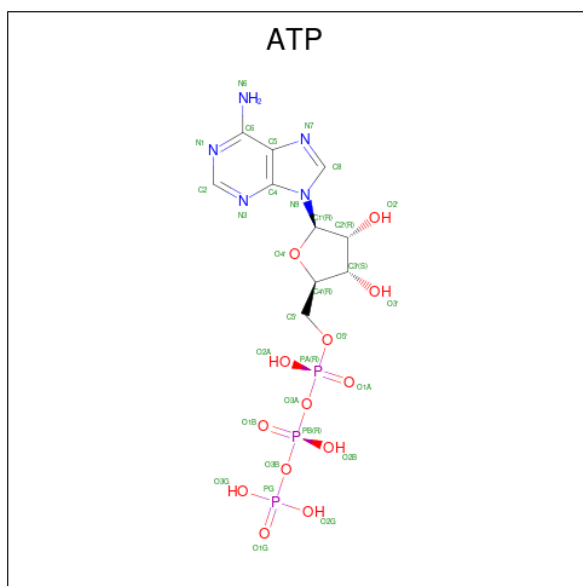
There are 4 unique types of molecules in this entry. The entry contains 11646 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-phosphofructokinase, muscle type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	748	Total	C	N	O	S	406	0	0
			5719	3583	1031	1068	37			
1	B	748	Total	C	N	O	S	420	0	0
			5719	3583	1031	1068	37			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- # ADP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

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- Diagram illustrating the Lewis structure of the phosphate ion (PO_4^{3-}). The central phosphorus atom (P) is bonded to four oxygen atoms (O). The bonds are as follows:
- Top: Single bond to O^- (labeled O3).
 - Bottom: Single bond to O^- (labeled O4).
 - Left: Single bond to O^- (labeled O2).
 - Right: Double bond to O (labeled O1).
- The phosphorus atom (P) has a positive charge (+). The oxygen atoms with single bonds have a negative charge ($-$).

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

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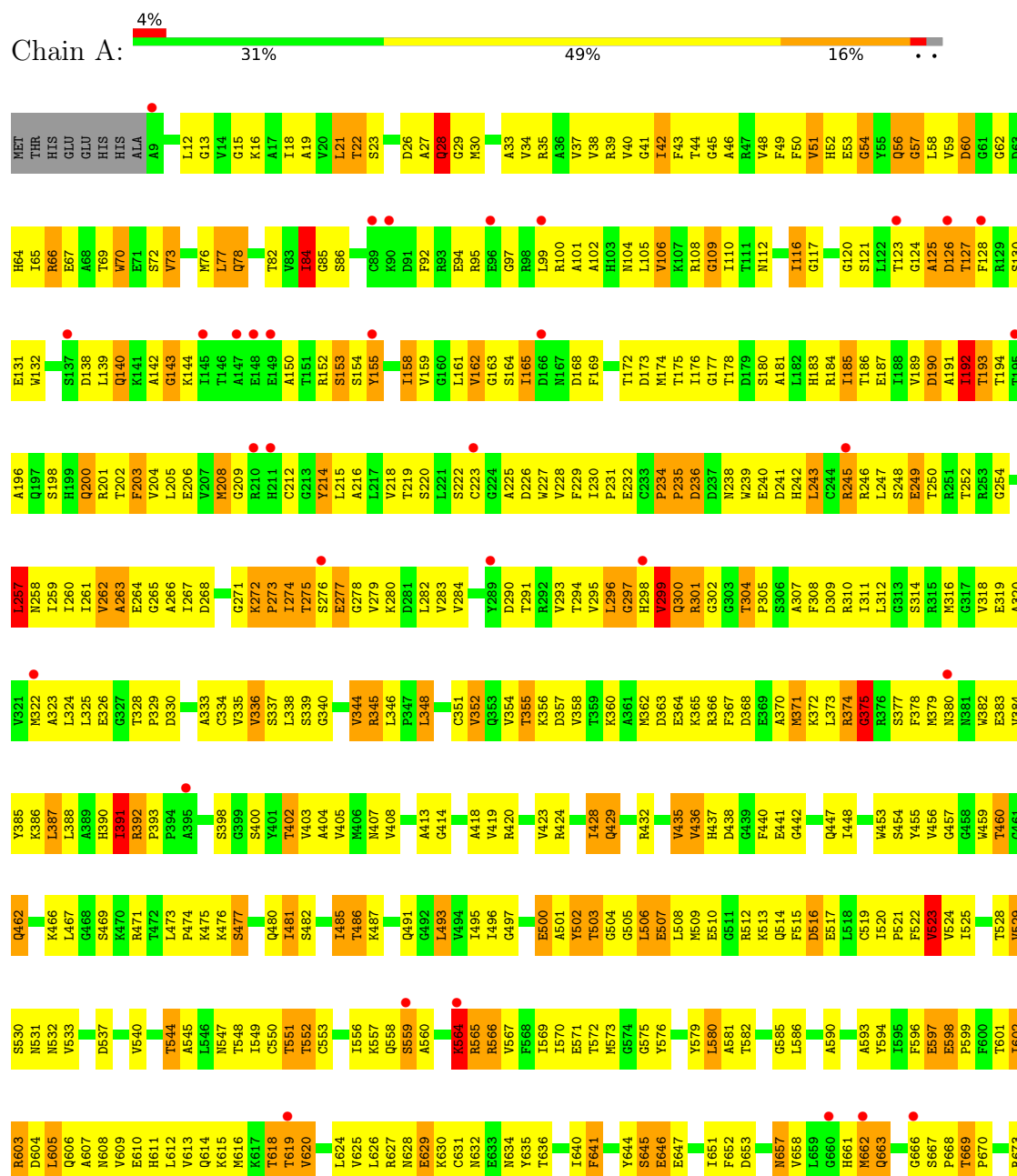
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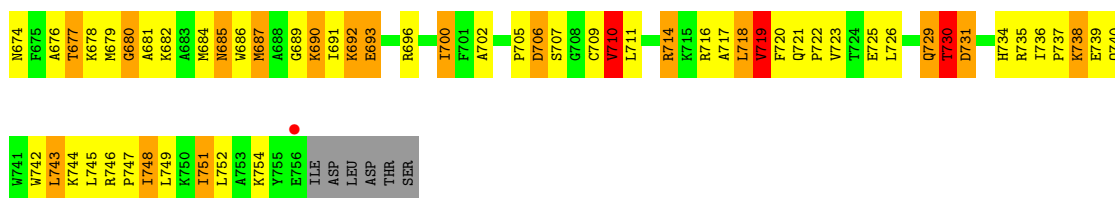
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

3 Residue-property plots

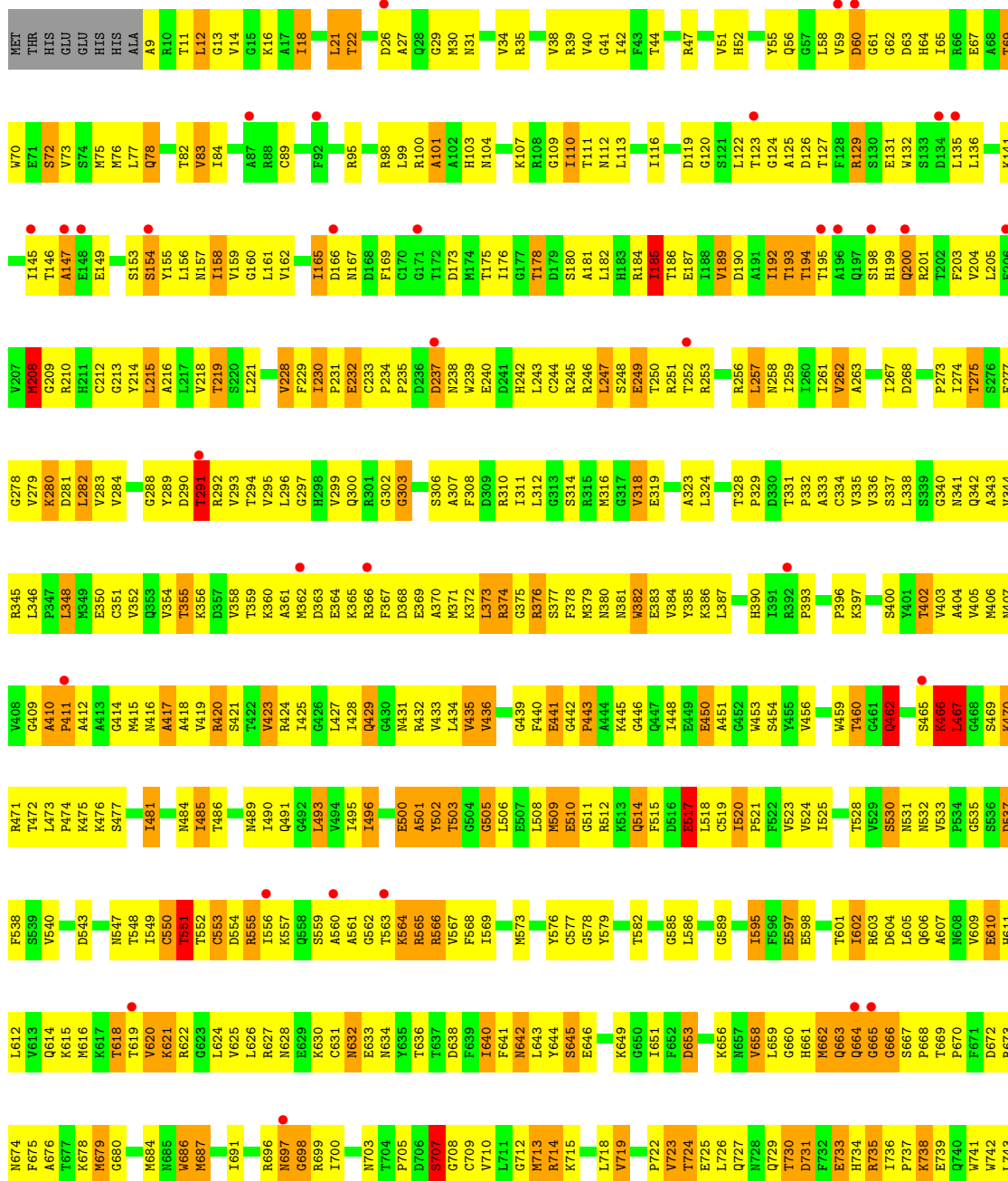
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 6-phosphofructokinase, muscle type





• Molecule 1: 6-phosphofructokinase, muscle type



K744	L745	R746	P747	I748	L749	K750	I751	L752	A753	K754	Y755	E756	ILE	ASP	LEU	ASP	THR	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	163.68Å 163.68Å 356.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.00 – 3.20 41.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.00-3.20) 99.9 (41.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.302 0.235 , 0.296	Depositor DCC
R_{free} test set	2362 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	81.9	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 117.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11646	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: PO4, ADP, 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	0.79	0/5819	1.24	67/7859 (0.9%)
1	B	0.79	4/5819 (0.1%)	1.21	59/7859 (0.8%)
All	All	0.79	4/11638 (0.0%)	1.22	126/15718 (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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	436	VAL	CA-CB	6.44	1.62	1.54
1	B	417	ALA	CA-CB	-5.72	1.44	1.53
1	B	185	ILE	CA-CB	5.23	1.62	1.54
1	B	423	VAL	CA-CB	-5.01	1.48	1.54

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	VAL	CA-C-N	-13.21	106.26	120.66
1	B	533	VAL	C-N-CA	-13.21	106.26	120.66
1	A	501	ALA	N-CA-C	-11.41	97.75	112.93
1	A	441	GLU	N-CA-C	-10.58	100.40	113.20
1	A	299	VAL	N-CA-C	-10.57	103.17	113.53
1	B	162	VAL	N-CA-C	10.07	121.67	107.37
1	A	598	GLU	CA-C-N	9.14	129.70	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	598	GLU	C-N-CA	9.14	129.70	119.83
1	B	686	TRP	N-CA-C	-8.40	102.07	111.14
1	B	520	ILE	CA-C-N	8.36	128.30	119.85
1	B	520	ILE	C-N-CA	8.36	128.30	119.85
1	A	234	PRO	CA-C-N	8.36	130.28	119.84
1	A	234	PRO	C-N-CA	8.36	130.28	119.84
1	B	738	LYS	N-CA-C	-8.21	98.33	110.48
1	A	709	CYS	N-CA-C	7.97	122.00	109.81
1	B	331	THR	CA-C-N	7.69	129.46	119.84
1	B	331	THR	C-N-CA	7.69	129.46	119.84
1	B	707	SER	N-CA-C	-7.68	103.94	113.38
1	A	523	VAL	CB-CA-C	-7.41	99.09	110.50
1	B	719	VAL	N-CA-C	7.28	120.25	108.97
1	A	249	GLU	N-CA-C	-7.24	102.19	111.02
1	B	505	GLY	N-CA-C	-6.88	96.87	113.18
1	B	467	LEU	N-CA-C	-6.78	105.14	113.41
1	B	462	GLN	N-CA-C	6.78	119.61	109.25
1	A	530	SER	N-CA-C	6.72	120.74	112.54
1	A	717	ALA	N-CA-C	6.72	119.39	109.24
1	B	52	HIS	N-CA-C	6.72	119.41	110.53
1	A	612	LEU	N-CA-C	-6.72	103.95	111.28
1	B	502	TYR	N-CA-C	-6.71	102.59	111.24
1	B	441	GLU	N-CA-C	-6.55	104.39	112.38
1	A	230	ILE	CA-C-N	6.53	128.00	119.84
1	A	230	ILE	C-N-CA	6.53	128.00	119.84
1	A	729	GLN	N-CA-C	-6.42	104.60	112.88
1	A	502	TYR	N-CA-C	-6.42	103.97	110.97
1	B	530	SER	N-CA-C	6.37	121.05	113.28
1	A	738	LYS	N-CA-C	-6.35	99.36	109.59
1	B	136	LEU	N-CA-C	-6.32	105.54	113.18
1	B	167	ASN	N-CA-C	-6.32	104.88	112.58
1	A	241	ASP	N-CA-C	-6.30	104.11	110.97
1	A	192	ILE	N-CA-C	-6.29	103.69	110.23
1	A	436	VAL	N-CA-C	6.27	116.89	107.80
1	B	610	GLU	N-CA-C	-6.23	105.53	113.01
1	A	710	VAL	N-CA-C	-6.20	99.42	108.11
1	B	621	LYS	N-CA-C	-6.20	105.73	113.55
1	A	162	VAL	N-CA-C	6.11	122.06	109.34
1	A	651	ILE	N-CA-C	6.07	117.54	110.62
1	B	633	GLU	N-CA-C	6.07	117.98	111.36
1	A	263	ALA	N-CA-C	-6.02	102.59	110.53
1	A	203	PHE	N-CA-C	6.00	118.03	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	692	LYS	N-CA-C	-5.99	104.38	111.03
1	B	733	GLU	N-CA-C	-5.97	104.47	110.97
1	A	702	ALA	N-CA-C	-5.96	99.49	108.96
1	B	663	GLN	N-CA-C	-5.96	107.83	114.62
1	B	517	GLU	N-CA-C	-5.90	104.93	111.36
1	A	322	MET	N-CA-C	-5.84	104.55	111.03
1	A	125	ALA	N-CA-C	-5.82	104.94	111.28
1	A	391	ILE	N-CA-C	-5.76	106.86	111.81
1	B	147	ALA	N-CA-C	-5.71	106.36	113.38
1	A	245	ARG	N-CA-C	-5.68	104.30	111.11
1	B	443	PRO	N-CA-C	-5.63	106.19	113.57
1	B	410	ALA	N-CA-C	-5.62	102.10	110.20
1	B	469	SER	N-CA-C	5.61	118.27	107.44
1	A	84	ILE	N-CA-C	-5.60	104.20	112.04
1	A	257	LEU	N-CA-C	5.60	118.08	110.35
1	B	429	GLN	N-CA-C	-5.57	105.98	112.89
1	B	474	PRO	N-CA-C	5.57	123.95	112.47
1	A	533	VAL	N-CA-C	5.54	113.40	108.63
1	A	429	GLN	N-CA-C	-5.53	106.53	113.28
1	A	150	ALA	N-CA-C	-5.51	106.75	112.93
1	B	376	ARG	N-CA-C	-5.49	104.70	111.40
1	B	230	ILE	CA-C-N	5.48	126.69	119.84
1	B	230	ILE	C-N-CA	5.48	126.69	119.84
1	A	185	ILE	CB-CA-C	-5.47	104.87	112.04
1	B	375	GLY	N-CA-C	5.47	117.47	110.96
1	B	291	THR	N-CA-C	5.46	122.43	110.80
1	B	653	ASP	N-CA-C	-5.44	101.93	110.36
1	A	667	SER	CA-C-N	5.42	125.68	119.83
1	A	667	SER	C-N-CA	5.42	125.68	119.83
1	B	501	ALA	N-CA-C	-5.40	106.82	113.41
1	A	520	ILE	CA-C-N	-5.40	114.78	120.66
1	A	520	ILE	C-N-CA	-5.40	114.78	120.66
1	A	262	VAL	CB-CA-C	-5.38	102.80	110.12
1	B	228	VAL	CB-CA-C	-5.36	103.85	111.19
1	A	368	ASP	N-CA-C	-5.35	105.53	111.36
1	A	603	ARG	N-CA-C	-5.33	105.58	111.71
1	B	101	ALA	N-CA-C	-5.32	105.39	111.14
1	A	375	GLY	N-CA-C	5.32	125.78	113.18
1	B	262	VAL	CB-CA-C	-5.31	104.08	110.99
1	A	477	SER	N-CA-C	5.30	118.81	111.71
1	A	272	LYS	CA-C-N	5.29	126.45	119.84
1	A	272	LYS	C-N-CA	5.29	126.45	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	743	LEU	N-CA-C	-5.29	106.52	112.87
1	B	640	ILE	CB-CA-C	-5.29	105.00	112.14
1	B	749	LEU	N-CA-C	-5.28	105.64	111.71
1	A	610	GLU	N-CA-C	-5.26	99.59	110.80
1	B	699	ARG	CA-C-N	-5.25	116.68	123.19
1	B	699	ARG	C-N-CA	-5.25	116.68	123.19
1	A	620	VAL	N-CA-C	5.24	117.17	109.63
1	A	355	THR	N-CA-C	-5.23	106.59	112.87
1	B	297	GLY	N-CA-C	5.23	120.75	111.02
1	A	300	GLN	N-CA-C	-5.21	105.60	111.28
1	A	274	ILE	N-CA-C	-5.21	100.96	108.87
1	A	310	ARG	N-CA-C	-5.20	105.53	111.14
1	B	496	ILE	N-CA-C	-5.19	101.10	108.58
1	B	162	VAL	CB-CA-C	-5.18	106.31	111.80
1	B	72	SER	N-CA-C	5.18	116.61	111.07
1	B	249	GLU	N-CA-C	-5.18	104.58	112.04
1	B	257	LEU	N-CA-C	5.17	116.84	108.41
1	A	116	ILE	CB-CA-C	-5.14	104.77	111.81
1	A	206	GLU	N-CA-C	-5.13	100.16	108.52
1	A	718	LEU	N-CA-C	-5.12	102.91	110.48
1	A	70	TRP	N-CA-C	-5.12	105.34	112.45
1	B	537	ASP	N-CA-C	-5.11	106.90	113.23
1	B	620	VAL	N-CA-C	5.11	116.16	109.21
1	B	417	ALA	N-CA-C	-5.11	104.98	111.11
1	A	345	ARG	N-CA-C	-5.10	100.20	108.52
1	B	746	ARG	CA-C-N	-5.08	114.50	119.64
1	B	746	ARG	C-N-CA	-5.08	114.50	119.64
1	A	719	VAL	N-CA-C	5.08	115.24	108.27
1	A	301	ARG	CA-C-N	-5.05	116.99	122.55
1	A	301	ARG	C-N-CA	-5.05	116.99	122.55
1	A	374	ARG	N-CA-C	-5.05	104.72	111.24
1	A	506	LEU	N-CA-C	-5.04	105.06	111.11
1	B	193	THR	N-CA-C	5.02	117.52	111.40
1	A	730	THR	N-CA-C	5.02	117.57	108.69
1	B	665	GLY	N-CA-C	-5.00	101.33	113.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	TYR	Sidechain

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	5719	0	5742	524	0
1	B	5719	0	5742	601	0
2	A	62	0	24	5	0
2	B	62	0	24	1	0
3	A	27	0	12	2	0
3	B	27	0	12	0	0
4	A	15	0	0	1	0
4	B	15	0	0	1	0
All	All	11646	0	11556	1116	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 53.

All (1116) 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:A:634:ASN:HD22	1:B:646:GLU:HG2	0.99	1.09
1:A:646:GLU:HG2	1:B:634:ASN:HD22	1.22	1.03
1:A:296:LEU:H	1:A:296:LEU:HD12	1.23	1.02
1:A:751:ILE:HD13	1:A:752:LEU:N	1.75	1.00
1:B:609:VAL:HG22	1:B:644:TYR:CE2	1.95	0.99
1:B:283:VAL:HG21	1:B:291:THR:HG21	1.45	0.98
1:A:634:ASN:ND2	1:B:646:GLU:HG2	1.79	0.98
1:B:35:ARG:HH11	1:B:77:LEU:HD13	1.25	0.96
1:B:567:VAL:HG22	1:B:616:MET:HE2	1.46	0.96
1:A:391:ILE:HD12	1:A:392:ARG:H	1.29	0.96
1:A:28:GLN:H	1:A:28:GLN:HE21	1.11	0.96
1:A:257:LEU:HD12	1:A:259:ILE:HD11	1.46	0.95
1:A:312:LEU:HD11	1:A:316:MET:HE2	1.46	0.93
1:B:514:GLN:H	1:B:514:GLN:HE21	1.12	0.91
1:A:334:CYS:SG	1:A:345:ARG:HB3	2.10	0.91
1:B:221:LEU:HD23	1:B:674:ASN:ND2	1.85	0.91
1:A:392:ARG:HB3	1:A:393:PRO:CA	2.01	0.90
1:B:39:ARG:HD2	1:B:70:TRP:CZ2	2.06	0.90
1:B:664:GLN:C	1:B:666:GLY:H	1.73	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ILE:HG22	1:A:261:ILE:CD1	2.01	0.90
1:B:734:HIS:O	1:B:736:ILE:HG23	1.72	0.90
1:B:159:VAL:HG23	1:B:324:LEU:HD23	1.55	0.89
1:A:392:ARG:HB3	1:A:393:PRO:HA	1.53	0.89
1:A:257:LEU:H	1:A:257:LEU:HD23	1.38	0.89
1:B:296:LEU:HD12	1:B:296:LEU:H	1.36	0.88
1:B:549:ILE:HD12	1:B:659:LEU:HD13	1.56	0.88
1:B:509:MET:SD	1:B:512:ARG:NH1	2.48	0.87
1:A:491:GLN:HB3	1:A:700:ILE:HD11	1.55	0.87
1:A:44:THR:HG21	1:A:325:LEU:HD11	1.56	0.86
1:A:18:ILE:HG22	1:A:112:ASN:HB2	1.57	0.86
1:B:520:ILE:HG22	1:B:700:ILE:HD11	1.56	0.86
1:B:416:ASN:OD1	1:B:466:LYS:HB2	1.74	0.86
1:B:275:THR:HG23	1:B:278:GLY:HA3	1.58	0.85
1:B:419:VAL:O	1:B:423:VAL:HG23	1.77	0.85
1:B:663:GLN:C	1:B:665:GLY:H	1.84	0.85
1:A:66:ARG:HA	1:A:66:ARG:NE	1.90	0.84
1:A:280:LYS:HG2	1:A:291:THR:CG2	2.07	0.84
1:A:392:ARG:CB	1:A:393:PRO:HA	2.06	0.84
1:B:221:LEU:HD23	1:B:674:ASN:HD22	1.37	0.84
1:B:120:GLY:O	1:B:123:THR:HG22	1.77	0.84
1:A:245:ARG:O	1:A:249:GLU:HG3	1.77	0.83
1:B:184:ARG:NH1	1:B:303:GLY:HA3	1.94	0.83
1:A:58:LEU:HG	1:A:101:ALA:HB1	1.59	0.83
1:B:348:LEU:O	1:B:352:VAL:HG23	1.77	0.82
1:A:165:ILE:O	1:A:215:LEU:HD11	1.78	0.82
1:B:595:ILE:HD13	1:B:595:ILE:H	1.43	0.81
1:A:646:GLU:HG2	1:B:634:ASN:HB2	1.62	0.81
1:B:35:ARG:HH12	1:B:77:LEU:HD22	1.42	0.81
1:B:618:THR:HG22	1:B:619:THR:N	1.95	0.81
1:A:40:VAL:HG21	1:A:318:VAL:HG22	1.61	0.81
1:B:664:GLN:C	1:B:666:GLY:N	2.38	0.81
1:A:296:LEU:H	1:A:296:LEU:CD1	1.94	0.81
1:B:514:GLN:HE21	1:B:514:GLN:N	1.78	0.81
1:A:391:ILE:HD11	2:A:765:ATP:O2G	1.79	0.81
1:B:459:TRP:H	1:B:459:TRP:CD1	1.99	0.80
1:B:208:MET:HB2	1:B:300:GLN:OE1	1.81	0.80
1:B:382:TRP:CZ2	1:B:386:LYS:HD2	2.16	0.80
1:B:641:PHE:CD2	1:B:656:LYS:HD3	2.17	0.80
1:A:491:GLN:HB3	1:A:700:ILE:CD1	2.10	0.80
1:A:243:LEU:HD12	1:A:243:LEU:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:O	1:A:366:ARG:N	2.15	0.80
1:A:391:ILE:HD11	2:A:765:ATP:PG	2.22	0.80
1:B:419:VAL:HG11	1:B:467:LEU:HD11	1.62	0.80
1:A:646:GLU:HG2	1:B:634:ASN:ND2	1.96	0.79
1:B:158:ILE:HD11	1:B:333:ALA:HB2	1.65	0.79
1:B:41:GLY:O	1:B:44:THR:HG22	1.81	0.79
1:B:35:ARG:NH1	1:B:77:LEU:HD13	1.96	0.79
1:A:646:GLU:CG	1:B:634:ASN:HB2	2.13	0.78
1:B:440:PHE:O	1:B:443:PRO:HD2	1.83	0.78
1:A:246:ARG:O	1:A:250:THR:HG22	1.84	0.78
1:A:268:ASP:HB3	1:A:274:ILE:HD11	1.65	0.78
1:B:509:MET:O	1:B:512:ARG:HB2	1.83	0.78
1:A:259:ILE:HG22	1:A:261:ILE:HD12	1.66	0.78
1:A:354:VAL:HA	1:A:357:ASP:OD2	1.83	0.78
1:A:280:LYS:HG2	1:A:291:THR:HG22	1.64	0.77
1:B:436:VAL:HG22	1:B:448:ILE:HD12	1.64	0.77
1:B:687:MET:HE3	1:B:687:MET:O	1.84	0.77
1:A:696:ARG:HG3	1:A:696:ARG:HH11	1.50	0.77
1:A:208:MET:HB2	1:A:300:GLN:OE1	1.84	0.77
1:B:658:VAL:HG12	1:B:658:VAL:O	1.83	0.77
1:A:172:THR:OG1	1:A:337:SER:HB2	1.83	0.76
1:A:380:ASN:O	1:A:384:VAL:HG23	1.85	0.76
1:A:609:VAL:C	1:A:611:HIS:H	1.93	0.76
1:B:350:GLU:O	1:B:354:VAL:HG23	1.85	0.76
1:B:441:GLU:OE2	1:B:472:THR:HG21	1.83	0.76
1:A:335:VAL:HG23	1:A:348:LEU:HG	1.67	0.76
1:B:470:LYS:HE2	1:B:471:ARG:H	1.50	0.76
1:A:312:LEU:O	1:A:316:MET:HG2	1.84	0.76
1:B:412:ALA:O	1:B:415:MET:HG3	1.86	0.76
1:A:391:ILE:HD12	1:A:392:ARG:N	2.01	0.76
1:B:257:LEU:HD12	1:B:259:ILE:HD11	1.68	0.76
1:A:120:GLY:O	1:A:123:THR:HG22	1.84	0.76
1:B:443:PRO:O	1:B:484:ASN:ND2	2.18	0.75
1:A:516:ASP:O	1:A:519:CYS:HB2	1.87	0.75
1:A:348:LEU:O	1:A:352:VAL:HG23	1.86	0.75
1:A:33:ALA:O	1:A:37:VAL:HG23	1.87	0.74
1:B:420:ARG:HH11	1:B:460:THR:HB	1.52	0.74
1:A:296:LEU:HD12	1:A:296:LEU:N	1.99	0.74
1:B:418:ALA:HB2	1:B:676:ALA:HB1	1.68	0.74
1:A:734:HIS:O	1:A:736:ILE:HG23	1.86	0.74
1:A:601:THR:HG22	1:A:604:ASP:OD2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ALA:HB2	1:A:624:LEU:HD23	1.69	0.74
1:A:551:THR:HG22	1:A:552:THR:N	2.00	0.74
1:B:618:THR:HG22	1:B:619:THR:H	1.52	0.74
1:B:642:ASN:HD22	1:B:642:ASN:N	1.85	0.74
1:B:69:THR:HG23	1:B:72:SER:HB3	1.70	0.73
1:A:192:ILE:HG22	1:A:193:THR:N	2.02	0.73
1:B:459:TRP:H	1:B:459:TRP:HD1	1.34	0.73
1:B:312:LEU:HD11	1:B:316:MET:HE2	1.72	0.72
1:B:40:VAL:HG22	1:B:751:ILE:HD11	1.71	0.72
1:A:120:GLY:HA2	1:A:123:THR:HG22	1.70	0.72
1:A:668:PRO:HG2	1:A:673:ARG:HE	1.54	0.72
1:A:548:THR:O	1:A:552:THR:HG23	1.88	0.72
1:B:124:GLY:HA2	1:B:127:THR:HG22	1.70	0.72
1:B:316:MET:HE1	1:B:338:LEU:N	2.04	0.72
1:A:364:GLU:C	1:A:366:ARG:H	1.97	0.72
1:A:275:THR:HG23	1:A:278:GLY:HA3	1.72	0.72
1:A:82:THR:HG21	1:A:86:SER:HB2	1.72	0.72
1:A:605:LEU:HD11	1:A:640:ILE:HD12	1.72	0.72
1:B:296:LEU:H	1:B:296:LEU:CD1	2.03	0.72
1:B:39:ARG:HD2	1:B:70:TRP:CE2	2.24	0.71
1:B:656:LYS:HG3	1:B:656:LYS:O	1.87	0.71
1:A:58:LEU:HD11	1:A:105:LEU:HD21	1.70	0.71
1:B:275:THR:O	1:B:279:VAL:HG23	1.90	0.71
1:A:220:SER:HB3	1:A:225:ALA:HB3	1.72	0.71
1:B:47:ARG:HD2	1:B:67:GLU:OE1	1.90	0.71
1:B:744:LYS:O	1:B:747:PRO:HD2	1.89	0.71
1:B:215:LEU:O	1:B:219:THR:CG2	2.38	0.71
1:B:281:ASP:O	1:B:284:VAL:N	2.24	0.71
1:B:595:ILE:HD12	1:B:746:ARG:NH1	2.05	0.71
1:A:387:LEU:HD23	1:A:428:ILE:HD13	1.71	0.71
1:B:159:VAL:HG23	1:B:324:LEU:CD2	2.20	0.71
1:B:283:VAL:HG23	1:B:284:VAL:N	2.05	0.71
1:B:528:THR:HG23	1:B:531:ASN:H	1.56	0.70
1:B:95:ARG:HA	1:B:98:ARG:HD2	1.72	0.70
1:B:663:GLN:O	1:B:665:GLY:N	2.24	0.70
1:B:567:VAL:CG2	1:B:616:MET:HE2	2.21	0.70
1:B:231:PRO:O	1:B:233:CYS:N	2.25	0.70
1:A:258:ASN:C	1:A:259:ILE:HD12	2.16	0.70
1:A:297:GLY:O	1:A:299:VAL:HG13	1.91	0.69
1:B:205:LEU:HD22	1:B:296:LEU:HD11	1.73	0.69
1:B:232:GLU:HG2	1:B:374:ARG:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASP:O	1:A:193:THR:HG22	1.92	0.69
1:B:69:THR:CG2	1:B:72:SER:HB3	2.22	0.69
1:A:275:THR:OG1	1:A:277:GLU:HG2	1.92	0.69
1:B:38:VAL:O	1:B:42:ILE:HG12	1.94	0.68
1:A:392:ARG:CB	1:A:393:PRO:CA	2.66	0.68
1:B:160:GLY:O	1:B:335:VAL:HG13	1.93	0.68
1:B:605:LEU:HD21	1:B:640:ILE:HD13	1.74	0.68
1:B:328:THR:HB	1:B:329:PRO:CD	2.23	0.68
1:B:679:MET:CE	1:B:718:LEU:HD11	2.22	0.68
1:A:521:PRO:HB3	1:A:707:SER:HB2	1.76	0.68
1:A:573:MET:HE3	1:A:661:HIS:HD2	1.56	0.68
1:A:69:THR:HG23	1:A:72:SER:H	1.57	0.68
1:A:280:LYS:HG3	1:A:293:VAL:HG23	1.76	0.68
1:B:205:LEU:HD23	1:B:294:THR:HB	1.74	0.68
1:B:247:LEU:HD23	1:B:258:ASN:ND2	2.08	0.68
1:B:481:ILE:C	1:B:481:ILE:HD12	2.18	0.68
1:B:35:ARG:NH1	1:B:77:LEU:HD22	2.08	0.68
1:B:61:GLY:O	1:B:63:ASP:N	2.26	0.68
1:B:158:ILE:HD11	1:B:333:ALA:CB	2.22	0.68
1:B:731:ASP:OD1	1:B:731:ASP:O	2.12	0.68
1:B:551:THR:HG22	1:B:552:THR:N	2.08	0.68
1:A:609:VAL:C	1:A:611:HIS:N	2.51	0.67
1:A:257:LEU:HD12	1:A:259:ILE:CD1	2.23	0.67
1:B:481:ILE:O	1:B:485:ILE:HG23	1.95	0.67
1:B:687:MET:HE1	1:B:691:ILE:HD11	1.77	0.67
1:B:435:VAL:CG1	1:B:467:LEU:HD21	2.24	0.67
1:A:268:ASP:HB3	1:A:274:ILE:CD1	2.24	0.67
1:B:281:ASP:O	1:B:283:VAL:N	2.27	0.67
1:B:493:LEU:HD23	1:B:495:ILE:HD11	1.77	0.67
1:A:27:ALA:O	1:A:30:MET:HG3	1.94	0.67
1:A:731:ASP:OD1	1:A:731:ASP:C	2.37	0.67
1:B:531:ASN:HD21	1:B:538:PHE:HA	1.59	0.67
1:A:51:VAL:HG12	1:A:51:VAL:O	1.95	0.66
1:A:259:ILE:HG22	1:A:261:ILE:HD11	1.76	0.66
1:A:262:VAL:HG12	1:A:263:ALA:O	1.95	0.66
1:B:456:VAL:O	1:B:459:TRP:CD1	2.49	0.66
1:B:609:VAL:HG13	1:B:644:TYR:CD2	2.30	0.66
1:B:247:LEU:CD2	1:B:258:ASN:HD22	2.08	0.66
1:B:403:VAL:HG21	1:B:684:MET:HE1	1.78	0.66
1:A:726:LEU:O	1:A:730:THR:HG22	1.95	0.66
1:A:711:LEU:HD11	1:A:718:LEU:HG	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:PRO:HG2	1:B:725:GLU:HB2	1.77	0.66
1:A:481:ILE:HG12	1:A:482:SER:N	2.10	0.66
1:B:595:ILE:HD13	1:B:595:ILE:N	2.11	0.66
1:A:601:THR:O	1:A:604:ASP:N	2.27	0.65
1:A:619:THR:HG23	1:A:620:VAL:H	1.61	0.65
1:B:502:TYR:OH	1:B:730:THR:HG21	1.96	0.65
1:B:65:ILE:HG22	1:B:65:ILE:O	1.95	0.65
1:B:510:GLU:O	1:B:512:ARG:N	2.29	0.65
1:A:297:GLY:O	1:A:299:VAL:N	2.30	0.65
1:B:402:THR:HG21	1:B:432:ARG:NH2	2.12	0.65
1:A:420:ARG:HA	1:A:456:VAL:HG11	1.78	0.65
1:B:247:LEU:HA	1:B:250:THR:HG22	1.79	0.65
1:A:528:THR:HG23	1:A:531:ASN:H	1.61	0.65
1:B:473:LEU:HD21	1:B:503:THR:HG22	1.78	0.65
1:A:228:VAL:HG12	1:A:229:PHE:N	2.12	0.65
1:B:419:VAL:HG21	1:B:467:LEU:HD12	1.79	0.65
1:B:495:ILE:HG22	1:B:501:ALA:HB1	1.79	0.65
1:A:419:VAL:O	1:A:423:VAL:HG23	1.97	0.65
1:B:39:ARG:CD	1:B:70:TRP:CE2	2.79	0.65
1:B:345:ARG:O	1:B:346:LEU:HD23	1.96	0.65
1:B:512:ARG:HH22	1:B:707:SER:HB2	1.60	0.65
1:B:514:GLN:H	1:B:514:GLN:NE2	1.90	0.65
1:A:66:ARG:HH21	1:A:108:ARG:NH2	1.95	0.64
1:A:333:ALA:HB1	1:A:348:LEU:HD12	1.78	0.64
1:A:387:LEU:HD22	1:A:428:ILE:HG21	1.79	0.64
1:A:646:GLU:CG	1:B:634:ASN:HD22	2.04	0.64
1:B:296:LEU:HD12	1:B:296:LEU:N	2.11	0.64
1:A:159:VAL:HG23	1:A:324:LEU:CD2	2.28	0.64
1:A:296:LEU:O	1:A:297:GLY:O	2.14	0.64
1:A:39:ARG:HD2	1:A:70:TRP:CE2	2.32	0.64
1:A:586:LEU:HD12	1:A:586:LEU:O	1.96	0.64
1:A:123:THR:O	1:A:127:THR:HG22	1.96	0.64
1:B:660:GLY:C	1:B:662:MET:H	2.06	0.64
1:B:21:LEU:O	1:B:21:LEU:HD23	1.97	0.64
1:B:112:ASN:OD1	1:B:157:ASN:HB2	1.98	0.64
1:B:247:LEU:HA	1:B:250:THR:CG2	2.28	0.64
1:B:387:LEU:CD2	1:B:428:ILE:HD13	2.27	0.64
1:B:726:LEU:HD23	1:B:729:GLN:OE1	1.97	0.64
1:A:475:LYS:O	1:A:477:SER:N	2.31	0.63
1:A:751:ILE:HD13	1:A:751:ILE:C	2.23	0.63
1:B:110:ILE:HD12	1:B:110:ILE:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:CYS:HA	1:B:597:GLU:OE2	1.97	0.63
1:A:569:ILE:HD12	1:A:641:PHE:HA	1.79	0.63
1:A:159:VAL:HG23	1:A:324:LEU:HD23	1.79	0.63
1:B:585:GLY:HA2	1:B:626:LEU:HD12	1.80	0.63
1:B:228:VAL:HG12	1:B:229:PHE:N	2.13	0.63
1:B:9:ALA:HB1	1:B:11:THR:HG22	1.80	0.63
1:B:334:CYS:HA	1:B:346:LEU:O	1.98	0.63
1:B:420:ARG:HG3	1:B:456:VAL:HB	1.81	0.63
1:B:612:LEU:O	1:B:616:MET:HG2	1.99	0.63
1:A:280:LYS:O	1:A:284:VAL:HG23	1.99	0.63
1:B:481:ILE:HD12	1:B:481:ILE:O	1.99	0.63
1:A:102:ALA:O	1:A:106:VAL:HG23	1.99	0.63
1:B:232:GLU:O	1:B:371:MET:HG2	1.98	0.63
1:B:182:LEU:HD11	1:B:218:VAL:HG11	1.80	0.63
1:B:193:THR:HG23	1:B:194:THR:N	2.13	0.63
1:B:428:ILE:HG13	1:B:453:TRP:HZ3	1.62	0.63
1:A:398:SER:C	1:A:400:SER:H	2.07	0.62
1:B:459:TRP:CD2	1:B:466:LYS:NZ	2.63	0.62
1:B:724:THR:HA	1:B:727:GLN:HE21	1.63	0.62
1:A:375:GLY:HA2	1:A:379:MET:HE3	1.80	0.62
1:A:503:THR:HG22	1:A:504:GLY:N	2.15	0.62
1:B:624:LEU:HD12	1:B:625:VAL:N	2.14	0.62
1:A:22:THR:HG21	1:A:82:THR:OG1	1.99	0.62
1:B:9:ALA:C	1:B:11:THR:H	2.06	0.62
1:B:101:ALA:HA	1:B:104:ASN:HD22	1.64	0.62
1:B:249:GLU:HA	1:B:252:THR:HG22	1.82	0.62
1:B:436:VAL:HG22	1:B:448:ILE:CD1	2.29	0.62
1:A:35:ARG:HD3	1:A:77:LEU:HD13	1.82	0.62
1:A:56:GLN:O	1:A:59:VAL:N	2.32	0.62
1:A:567:VAL:HG23	1:A:616:MET:HE2	1.80	0.62
1:A:202:THR:HG22	1:A:202:THR:O	2.00	0.61
1:A:496:ILE:CD1	1:A:525:ILE:HD12	2.30	0.61
1:B:605:LEU:HD11	1:B:640:ILE:HD12	1.82	0.61
1:B:669:THR:O	1:B:673:ARG:HG3	2.00	0.61
1:A:49:PHE:CD1	1:A:110:ILE:HD11	2.34	0.61
1:A:95:ARG:C	1:A:97:GLY:H	2.07	0.61
1:B:76:MET:HE3	1:B:83:VAL:HB	1.83	0.61
1:A:565:ARG:HG2	1:A:565:ARG:HH21	1.65	0.61
1:B:376:ARG:HH21	1:B:376:ARG:HB3	1.65	0.61
1:A:185:ILE:HD11	1:A:215:LEU:HD23	1.82	0.61
1:B:514:GLN:N	1:B:514:GLN:NE2	2.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:ASN:O	1:B:636:THR:HG23	2.01	0.61
1:A:50:PHE:CE2	1:A:84:ILE:HD11	2.36	0.61
1:A:259:ILE:CG2	1:A:261:ILE:HD11	2.31	0.61
1:A:19:ALA:HA	1:A:49:PHE:O	2.01	0.61
1:B:283:VAL:HG23	1:B:284:VAL:H	1.65	0.61
1:B:481:ILE:HD11	1:B:518:LEU:HD21	1.82	0.61
1:B:485:ILE:HG12	1:B:517:GLU:HB3	1.82	0.61
1:B:126:ASP:HB2	1:B:348:LEU:HD22	1.81	0.61
1:A:35:ARG:HH12	1:A:752:LEU:HD13	1.66	0.60
1:B:228:VAL:HG12	1:B:229:PHE:H	1.64	0.60
1:B:668:PRO:HB2	1:B:673:ARG:HG2	1.83	0.60
1:A:722:PRO:HG2	1:A:725:GLU:HG3	1.82	0.60
1:B:601:THR:O	1:B:603:ARG:N	2.34	0.60
1:A:308:PHE:CZ	1:A:312:LEU:HD22	2.36	0.60
1:B:307:ALA:H	1:B:547:ASN:HD21	1.47	0.60
1:B:495:ILE:CG2	1:B:501:ALA:HB1	2.32	0.60
1:B:679:MET:HE1	1:B:718:LEU:HD11	1.83	0.60
1:B:281:ASP:O	1:B:282:LEU:C	2.43	0.60
1:A:609:VAL:O	1:A:611:HIS:N	2.30	0.60
1:B:627:ARG:NH2	1:B:636:THR:HA	2.17	0.60
1:A:153:SER:C	1:A:155:TYR:H	2.08	0.60
1:B:604:ASP:O	1:B:607:ALA:N	2.33	0.60
1:A:52:HIS:HA	1:A:84:ILE:O	2.02	0.60
1:B:333:ALA:HB1	1:B:348:LEU:HD12	1.84	0.60
1:A:99:LEU:HD12	1:A:100:ARG:N	2.17	0.60
1:A:183:HIS:O	1:A:187:GLU:HG3	2.01	0.60
1:A:28:GLN:H	1:A:28:GLN:NE2	1.93	0.59
1:A:590:ALA:HA	1:A:624:LEU:HB3	1.83	0.59
1:A:120:GLY:CA	1:A:123:THR:HG22	2.32	0.59
1:A:280:LYS:HG2	1:A:291:THR:HG21	1.83	0.59
1:B:18:ILE:HD12	1:B:324:LEU:HD12	1.84	0.59
1:B:185:ILE:HD12	1:B:219:THR:HB	1.85	0.59
1:B:425:ILE:O	1:B:429:GLN:HG3	2.02	0.59
1:B:456:VAL:HA	1:B:459:TRP:NE1	2.17	0.59
1:A:78:GLN:N	1:A:78:GLN:OE1	2.35	0.59
1:B:185:ILE:O	1:B:189:VAL:HG23	2.00	0.59
1:B:459:TRP:CD1	1:B:459:TRP:N	2.64	0.59
1:A:66:ARG:HA	1:A:66:ARG:CZ	2.32	0.59
1:A:593:ALA:HA	1:A:626:LEU:O	2.02	0.59
1:B:485:ILE:C	1:B:485:ILE:HD12	2.28	0.59
1:B:562:GLY:C	1:B:564:LYS:H	2.08	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:MET:HE1	1:A:705:PRO:HA	1.85	0.59
1:B:416:ASN:HB3	1:B:459:TRP:HB3	1.84	0.59
1:B:675:PHE:HA	1:B:678:LYS:HE2	1.85	0.59
2:A:763:ATP:O2A	2:A:763:ATP:O2B	2.21	0.59
1:B:193:THR:C	1:B:195:THR:H	2.11	0.59
1:B:404:ALA:HB2	1:B:490:ILE:HD12	1.84	0.59
1:B:532:ASN:O	1:B:737:PRO:HD3	2.02	0.59
1:B:551:THR:O	1:B:552:THR:C	2.46	0.59
1:B:595:ILE:HD12	1:B:746:ARG:HH12	1.65	0.59
1:B:166:ASP:OD1	1:B:209:GLY:HA2	2.02	0.58
1:B:700:ILE:HG13	1:B:700:ILE:O	2.02	0.58
1:B:314:SER:O	1:B:318:VAL:HG23	2.03	0.58
1:B:481:ILE:HD11	1:B:518:LEU:CD2	2.33	0.58
1:A:459:TRP:HA	1:A:462:GLN:HG3	1.85	0.58
1:B:306:SER:O	1:B:310:ARG:HG3	2.04	0.58
1:B:566:ARG:O	1:B:616:MET:HE1	2.03	0.58
1:A:267:ILE:HA	1:A:273:PRO:HA	1.84	0.58
1:B:713:MET:HG3	1:B:718:LEU:HD12	1.83	0.58
1:A:726:LEU:HD23	1:A:729:GLN:OE1	2.03	0.58
1:B:416:ASN:OD1	1:B:466:LYS:CB	2.49	0.58
1:B:535:GLY:O	1:B:712:GLY:HA3	2.03	0.58
1:B:289:TYR:C	1:B:291:THR:H	2.11	0.58
1:B:215:LEU:O	1:B:219:THR:HG22	2.03	0.58
1:B:231:PRO:C	1:B:233:CYS:H	2.11	0.58
1:B:216:ALA:O	1:B:219:THR:HG23	2.04	0.57
1:A:646:GLU:HG2	1:B:634:ASN:CB	2.32	0.57
1:B:319:GLU:OE2	1:B:345:ARG:NE	2.37	0.57
1:B:21:LEU:HD23	1:B:21:LEU:C	2.28	0.57
1:A:153:SER:O	1:A:155:TYR:N	2.26	0.57
1:A:268:ASP:CB	1:A:274:ILE:HD11	2.34	0.57
1:A:524:VAL:CG1	1:A:710:VAL:HG22	2.34	0.57
1:B:39:ARG:HG3	1:B:39:ARG:HH11	1.69	0.57
1:B:369:GLU:O	1:B:373:LEU:HB2	2.03	0.57
1:B:632:ASN:OD1	1:B:632:ASN:C	2.47	0.57
1:A:15:GLY:O	1:A:16:LYS:HG2	2.05	0.57
1:B:158:ILE:HD13	1:B:158:ILE:H	1.70	0.57
1:B:323:ALA:HA	1:B:345:ARG:HH12	1.70	0.57
1:A:116:ILE:HG12	1:A:161:LEU:HD13	1.86	0.57
1:A:219:THR:O	1:A:223:CYS:SG	2.57	0.57
1:A:243:LEU:HD12	1:A:247:LEU:HD12	1.87	0.57
1:B:40:VAL:HG21	1:B:318:VAL:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:VAL:HB	1:B:467:LEU:HD21	1.87	0.57
1:A:42:ILE:HD13	1:A:48:VAL:HG23	1.87	0.57
1:A:371:MET:SD	1:A:378:PHE:CE2	2.98	0.56
1:B:611:HIS:CE1	1:B:754:LYS:HB3	2.40	0.56
1:A:50:PHE:O	1:A:51:VAL:HG23	2.05	0.56
1:B:372:LYS:HA	1:B:379:MET:HE1	1.85	0.56
1:B:387:LEU:HD22	1:B:428:ILE:HD13	1.86	0.56
1:A:364:GLU:C	1:A:366:ARG:N	2.62	0.56
1:A:564:LYS:HE2	1:A:564:LYS:HA	1.86	0.56
1:A:523:VAL:HG22	1:A:686:TRP:CZ3	2.39	0.56
1:B:485:ILE:HD12	1:B:485:ILE:O	2.05	0.56
1:B:649:LYS:C	1:B:651:ILE:H	2.13	0.56
1:A:682:LYS:HG2	1:A:718:LEU:HD23	1.87	0.56
1:B:145:ILE:C	1:B:147:ALA:H	2.13	0.56
1:B:169:PHE:CE2	1:B:351:CYS:HB3	2.40	0.56
1:B:609:VAL:HG13	1:B:644:TYR:HD2	1.70	0.56
1:B:669:THR:HB	1:B:670:PRO:HD2	1.86	0.56
1:A:714:ARG:HE	1:A:714:ARG:HA	1.71	0.56
1:B:221:LEU:CD2	1:B:674:ASN:HD22	2.15	0.56
1:B:687:MET:HE3	1:B:687:MET:C	2.30	0.56
1:A:352:VAL:HA	1:A:355:THR:HG22	1.86	0.56
1:B:247:LEU:HD23	1:B:258:ASN:HD22	1.70	0.56
1:B:731:ASP:OD1	1:B:731:ASP:C	2.47	0.56
1:A:471:ARG:HB3	1:A:500:GLU:HG3	1.87	0.56
1:A:532:ASN:O	1:A:737:PRO:HD3	2.05	0.56
1:B:556:ILE:HG22	1:B:568:PHE:CD2	2.40	0.56
1:B:543:ASP:HB3	1:B:672:ASP:OD2	2.06	0.56
1:B:275:THR:HG23	1:B:278:GLY:CA	2.32	0.56
1:A:679:MET:HE3	1:A:718:LEU:HD11	1.89	0.55
1:B:292:ARG:O	1:B:293:VAL:HG23	2.06	0.55
1:B:433:VAL:C	1:B:434:LEU:HD12	2.30	0.55
1:A:26:ASP:O	1:A:301:ARG:NH1	2.39	0.55
1:A:177:GLY:N	1:A:309:ASP:OD1	2.37	0.55
1:B:235:PRO:HD2	1:B:267:ILE:O	2.07	0.55
1:B:611:HIS:HE1	1:B:754:LYS:HB3	1.70	0.55
1:A:138:ASP:C	1:A:140:GLN:H	2.14	0.55
1:A:686:TRP:CZ3	1:A:687:MET:HG2	2.41	0.55
1:B:124:GLY:CA	1:B:127:THR:HG22	2.37	0.55
1:B:190:ASP:O	1:B:194:THR:HG23	2.07	0.55
1:B:745:LEU:O	1:B:748:ILE:HG12	2.06	0.55
1:A:391:ILE:HD12	1:A:391:ILE:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:VAL:O	1:A:497:GLY:HA3	2.06	0.55
1:A:101:ALA:HA	1:A:104:ASN:HD22	1.71	0.55
1:B:708:GLY:O	1:B:723:VAL:HG22	2.05	0.55
1:A:168:ASP:OD2	1:A:169:PHE:N	2.39	0.55
1:A:335:VAL:CG2	1:A:348:LEU:HG	2.37	0.55
1:A:605:LEU:HD21	1:A:640:ILE:HD13	1.88	0.55
1:B:299:VAL:HG23	1:B:300:GLN:N	2.22	0.55
1:A:294:THR:HG22	1:A:295:VAL:N	2.22	0.55
1:A:696:ARG:HG3	1:A:696:ARG:NH1	2.21	0.55
1:B:257:LEU:O	1:B:257:LEU:HG	2.06	0.55
1:B:281:ASP:C	1:B:283:VAL:N	2.63	0.55
1:B:535:GLY:O	1:B:714:ARG:HD2	2.06	0.55
1:B:537:ASP:HB3	1:B:741:TRP:NE1	2.20	0.55
1:A:402:THR:HB	1:A:432:ARG:HB3	1.89	0.55
1:A:569:ILE:HG12	1:A:625:VAL:HB	1.88	0.55
1:A:627:ARG:NH2	1:A:636:THR:HA	2.21	0.55
1:A:645:SER:O	1:A:646:GLU:C	2.49	0.55
1:A:646:GLU:HG3	1:B:634:ASN:HB2	1.86	0.55
1:A:726:LEU:O	1:A:730:THR:CG2	2.54	0.55
1:B:63:ASP:C	1:B:65:ILE:H	2.15	0.55
1:A:95:ARG:C	1:A:97:GLY:N	2.65	0.55
1:A:596:PHE:C	1:A:596:PHE:CD2	2.84	0.55
1:B:160:GLY:O	1:B:335:VAL:HA	2.07	0.55
1:B:240:GLU:N	1:B:240:GLU:OE1	2.40	0.55
1:B:441:GLU:OE2	1:B:472:THR:CG2	2.54	0.55
1:A:387:LEU:CD2	1:A:428:ILE:HG21	2.37	0.54
1:B:18:ILE:HD12	1:B:324:LEU:CD1	2.38	0.54
1:B:641:PHE:CG	1:B:656:LYS:HD3	2.42	0.54
1:A:275:THR:HG23	1:A:278:GLY:CA	2.37	0.54
1:A:275:THR:O	1:A:279:VAL:HG23	2.07	0.54
1:B:402:THR:HG23	1:B:491:GLN:HE21	1.72	0.54
1:A:551:THR:CG2	1:A:552:THR:N	2.68	0.54
1:B:471:ARG:HB2	1:B:500:GLU:HG2	1.90	0.54
1:A:271:GLY:O	1:A:273:PRO:HD3	2.07	0.54
1:B:9:ALA:C	1:B:11:THR:N	2.65	0.54
1:B:47:ARG:HD2	1:B:67:GLU:CD	2.32	0.54
1:B:565:ARG:HG3	1:B:565:ARG:HH11	1.73	0.54
1:A:231:PRO:O	1:A:234:PRO:HD3	2.07	0.54
1:A:271:GLY:O	1:A:273:PRO:CD	2.55	0.54
1:A:513:LYS:HB2	1:A:514:GLN:NE2	2.23	0.54
1:A:679:MET:O	1:A:681:ALA:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:PRO:HB2	1:B:268:ASP:C	2.33	0.54
1:B:523:VAL:HG22	1:B:686:TRP:CZ3	2.42	0.54
1:B:564:LYS:O	1:B:565:ARG:C	2.50	0.54
1:A:204:VAL:HG12	1:A:204:VAL:O	2.07	0.54
1:A:340:GLY:HA2	1:A:716:ARG:HA	1.90	0.54
1:A:403:VAL:HG12	1:A:404:ALA:N	2.23	0.54
1:B:609:VAL:HA	1:B:644:TYR:HE2	1.72	0.54
1:A:53:GLU:O	1:A:54:GLY:O	2.26	0.54
1:A:328:THR:C	1:A:330:ASP:H	2.16	0.54
1:B:119:ASP:OD1	1:B:120:GLY:N	2.38	0.54
1:B:267:ILE:HA	1:B:273:PRO:HA	1.88	0.54
1:A:29:GLY:HA3	1:A:176:ILE:CG2	2.38	0.54
1:A:721:GLN:NE2	1:A:726:LEU:HD21	2.23	0.54
1:B:41:GLY:C	1:B:44:THR:HG22	2.33	0.54
1:B:376:ARG:CB	1:B:376:ARG:NH2	2.70	0.54
1:B:420:ARG:HH11	1:B:460:THR:CB	2.20	0.54
1:B:175:THR:O	1:B:178:THR:HG22	2.08	0.54
1:B:364:GLU:O	1:B:366:ARG:N	2.41	0.54
1:B:382:TRP:CE2	1:B:386:LYS:HD2	2.43	0.54
1:B:605:LEU:HG	1:B:643:LEU:HD23	1.90	0.54
1:A:722:PRO:HG2	1:A:725:GLU:CG	2.37	0.53
1:B:726:LEU:O	1:B:729:GLN:HB2	2.08	0.53
1:B:11:THR:O	1:B:13:GLY:N	2.42	0.53
1:B:409:GLY:HA2	1:B:471:ARG:HB3	1.89	0.53
1:A:436:VAL:HG13	1:A:442:GLY:HA3	1.90	0.53
1:A:567:VAL:CG2	1:A:616:MET:HE2	2.39	0.53
1:A:35:ARG:HA	1:A:73:VAL:HG11	1.89	0.53
1:A:375:GLY:HA2	1:A:379:MET:CE	2.39	0.53
1:A:435:VAL:HG13	1:A:467:LEU:CD2	2.39	0.53
1:B:21:LEU:HD12	1:B:51:VAL:HG11	1.90	0.53
1:B:34:VAL:O	1:B:38:VAL:HG23	2.07	0.53
1:B:185:ILE:O	1:B:185:ILE:HG12	2.08	0.53
1:B:667:SER:OG	1:B:668:PRO:HD2	2.08	0.53
1:B:679:MET:HE3	1:B:718:LEU:HD11	1.88	0.53
1:A:189:VAL:O	1:A:193:THR:HB	2.09	0.53
1:A:738:LYS:O	1:A:739:GLU:HB2	2.09	0.53
1:A:748:ILE:CG1	1:A:749:LEU:N	2.71	0.53
1:B:124:GLY:HA2	1:B:127:THR:CG2	2.38	0.53
1:B:182:LEU:CD1	1:B:218:VAL:HG11	2.38	0.53
1:B:283:VAL:CG2	1:B:284:VAL:N	2.72	0.53
1:B:402:THR:HG21	1:B:432:ARG:HH21	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:VAL:O	1:A:60:ASP:O	2.26	0.53
1:A:120:GLY:O	1:A:123:THR:CG2	2.54	0.53
1:A:500:GLU:OE2	1:A:735:ARG:NH2	2.40	0.53
1:A:711:LEU:HD22	1:A:720:PHE:CZ	2.44	0.53
1:B:184:ARG:HA	1:B:187:GLU:OE2	2.09	0.53
1:B:231:PRO:C	1:B:233:CYS:N	2.67	0.53
1:B:316:MET:HE1	1:B:337:SER:C	2.33	0.53
1:B:407:ASN:O	1:B:439:GLY:HA2	2.09	0.53
1:B:549:ILE:O	1:B:553:CYS:HB2	2.09	0.53
1:B:679:MET:O	1:B:680:GLY:C	2.51	0.53
1:B:709:CYS:HA	1:B:722:PRO:HA	1.89	0.53
1:A:124:GLY:O	1:A:127:THR:HG23	2.09	0.53
1:B:84:ILE:HD12	1:B:84:ILE:N	2.24	0.53
1:B:213:GLY:HA3	1:B:230:ILE:HG22	1.89	0.53
1:A:35:ARG:HD3	1:A:77:LEU:CD1	2.38	0.53
1:A:57:GLY:HA2	1:A:64:HIS:CD2	2.44	0.53
1:A:130:SER:C	1:A:132:TRP:H	2.17	0.53
1:A:436:VAL:CG1	1:A:442:GLY:HA3	2.38	0.53
1:A:572:THR:O	1:A:629:GLU:HB3	2.08	0.53
1:B:407:ASN:HA	1:B:496:ILE:O	2.09	0.53
1:B:738:LYS:O	1:B:739:GLU:HB2	2.08	0.53
1:A:751:ILE:HD13	1:A:752:LEU:H	1.67	0.53
1:B:319:GLU:HG2	1:B:343:ALA:HB1	1.90	0.53
1:B:470:LYS:HG3	1:B:472:THR:HG23	1.90	0.53
1:A:746:ARG:N	1:A:747:PRO:HD2	2.24	0.52
1:B:41:GLY:O	1:B:44:THR:CG2	2.53	0.52
1:A:265:GLY:O	1:A:267:ILE:HG23	2.08	0.52
1:A:580:LEU:O	1:A:581:ALA:C	2.51	0.52
1:B:257:LEU:HD23	1:B:257:LEU:H	1.74	0.52
1:B:569:ILE:HD12	1:B:641:PHE:HA	1.91	0.52
1:B:358:VAL:HA	1:B:373:LEU:HD13	1.91	0.52
1:B:402:THR:CB	1:B:432:ARG:HH21	2.22	0.52
1:A:239:TRP:CD1	1:A:240:GLU:N	2.78	0.52
1:A:379:MET:O	1:A:383:GLU:HG2	2.09	0.52
1:A:509:MET:O	1:A:512:ARG:HB2	2.09	0.52
1:B:560:ALA:C	1:B:622:ARG:HH22	2.18	0.52
1:A:360:LYS:O	1:A:363:ASP:N	2.42	0.52
1:A:440:PHE:C	1:A:442:GLY:N	2.65	0.52
1:A:604:ASP:O	1:A:607:ALA:N	2.43	0.52
1:A:165:ILE:N	1:A:165:ILE:HD13	2.23	0.52
1:A:371:MET:CE	1:A:382:TRP:CD1	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:ASP:OD1	1:A:706:ASP:N	2.41	0.52
1:A:228:VAL:CG1	1:A:229:PHE:N	2.71	0.52
1:A:380:ASN:HD22	1:A:678:LYS:HE2	1.75	0.52
1:A:475:LYS:C	1:A:477:SER:H	2.18	0.52
1:A:485:ILE:O	1:A:485:ILE:HG13	2.08	0.52
1:B:364:GLU:C	1:B:366:ARG:H	2.17	0.52
1:B:642:ASN:N	1:B:642:ASN:ND2	2.53	0.52
1:A:185:ILE:O	1:A:189:VAL:HG23	2.10	0.52
1:A:437:HIS:O	1:A:438:ASP:HB2	2.10	0.52
1:A:506:LEU:CD2	1:A:723:VAL:HB	2.39	0.52
1:B:126:ASP:O	1:B:129:ARG:HG3	2.09	0.52
1:A:247:LEU:HA	1:A:250:THR:CG2	2.40	0.52
1:A:374:ARG:HG2	1:A:378:PHE:CD2	2.45	0.51
1:A:689:GLY:O	1:A:692:LYS:N	2.43	0.51
1:B:578:GLY:H	1:B:597:GLU:CD	2.18	0.51
1:A:120:GLY:C	1:A:123:THR:HG22	2.35	0.51
1:A:440:PHE:C	1:A:442:GLY:H	2.14	0.51
1:A:613:VAL:C	1:A:615:LYS:H	2.17	0.51
1:B:55:TYR:O	1:B:58:LEU:N	2.42	0.51
1:B:419:VAL:HG11	1:B:467:LEU:CD1	2.37	0.51
1:B:459:TRP:O	1:B:462:GLN:HG3	2.09	0.51
1:B:664:GLN:O	1:B:666:GLY:N	2.43	0.51
1:B:687:MET:O	1:B:691:ILE:HG12	2.10	0.51
1:A:316:MET:HE1	1:A:338:LEU:N	2.25	0.51
1:B:9:ALA:HB3	1:B:12:LEU:H	1.76	0.51
1:B:214:TYR:CZ	1:B:218:VAL:HG21	2.46	0.51
1:B:713:MET:HG3	1:B:718:LEU:CD1	2.40	0.51
1:A:139:LEU:O	1:A:143:GLY:HA3	2.10	0.51
1:A:475:LYS:C	1:A:477:SER:N	2.69	0.51
1:A:679:MET:O	1:A:680:GLY:C	2.51	0.51
1:B:262:VAL:HG12	1:B:263:ALA:O	2.10	0.51
1:A:39:ARG:HD2	1:A:70:TRP:CZ2	2.44	0.51
1:A:557:LYS:O	1:A:558:GLN:NE2	2.44	0.51
1:A:748:ILE:HG12	1:A:749:LEU:N	2.26	0.51
1:B:153:SER:O	1:B:155:TYR:N	2.43	0.51
1:B:212:CYS:HA	1:B:232:GLU:OE2	2.11	0.51
1:A:33:ALA:HB3	1:A:116:ILE:HD13	1.92	0.51
1:B:110:ILE:H	1:B:110:ILE:CD1	2.22	0.51
1:B:624:LEU:HD12	1:B:625:VAL:H	1.73	0.51
1:A:601:THR:O	1:A:601:THR:HG23	2.09	0.51
1:B:11:THR:HA	1:B:14:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:SER:C	1:B:155:TYR:N	2.68	0.51
1:B:515:PHE:N	1:B:515:PHE:CD1	2.78	0.51
1:A:235:PRO:O	1:A:236:ASP:C	2.53	0.51
1:B:214:TYR:C	1:B:216:ALA:H	2.18	0.51
1:B:234:PRO:HG3	1:B:367:PHE:CZ	2.45	0.51
1:B:378:PHE:C	1:B:378:PHE:CD2	2.89	0.51
1:B:615:LYS:HB3	1:B:620:VAL:HG21	1.93	0.51
1:A:500:GLU:CD	1:A:735:ARG:HH21	2.19	0.51
1:B:415:MET:O	1:B:419:VAL:HG23	2.10	0.51
1:B:551:THR:O	1:B:554:ASP:N	2.42	0.51
1:A:239:TRP:CD1	1:A:239:TRP:C	2.89	0.51
2:A:763:ATP:O5'	2:A:763:ATP:H8	1.93	0.51
1:B:311:ILE:HG23	1:B:586:LEU:HD23	1.93	0.51
1:B:595:ILE:N	1:B:595:ILE:CD1	2.74	0.51
1:A:227:TRP:CD1	1:A:228:VAL:N	2.79	0.50
1:A:259:ILE:CG2	1:A:261:ILE:CD1	2.82	0.50
1:A:517:GLU:C	1:A:519:CYS:H	2.18	0.50
1:B:328:THR:HB	1:B:329:PRO:HD2	1.93	0.50
1:B:435:VAL:HG22	1:B:451:ALA:HB2	1.92	0.50
1:B:665:GLY:O	1:B:666:GLY:O	2.28	0.50
1:A:66:ARG:HH21	1:A:108:ARG:HH22	1.56	0.50
1:A:214:TYR:O	1:A:218:VAL:HG23	2.12	0.50
1:B:165:ILE:HD11	1:B:208:MET:HG2	1.93	0.50
1:A:165:ILE:H	1:A:165:ILE:CD1	2.24	0.50
1:B:214:TYR:C	1:B:216:ALA:N	2.69	0.50
1:B:435:VAL:CB	1:B:467:LEU:HD21	2.41	0.50
1:B:459:TRP:CG	1:B:466:LYS:HZ3	2.27	0.50
1:B:731:ASP:OD2	1:B:734:HIS:HD2	1.94	0.50
1:A:392:ARG:HB2	1:A:393:PRO:HA	1.87	0.50
1:A:662:MET:O	1:A:663:GLN:C	2.54	0.50
1:B:248:SER:O	1:B:252:THR:HG22	2.10	0.50
1:B:294:THR:HG22	1:B:295:VAL:N	2.27	0.50
1:B:568:PHE:CD1	1:B:568:PHE:N	2.78	0.50
1:B:729:GLN:O	1:B:738:LYS:HG3	2.12	0.50
1:A:371:MET:SD	1:A:378:PHE:HE2	2.35	0.50
1:A:576:TYR:HD2	1:A:596:PHE:CD1	2.28	0.50
1:A:601:THR:O	1:A:603:ARG:N	2.44	0.50
1:B:364:GLU:C	1:B:366:ARG:N	2.70	0.50
1:A:189:VAL:HG22	1:A:205:LEU:CD1	2.42	0.50
1:A:596:PHE:O	1:A:598:GLU:N	2.45	0.50
1:B:423:VAL:HG12	1:B:427:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:ALA:C	1:B:562:GLY:H	2.20	0.50
1:B:601:THR:O	1:B:602:ILE:C	2.54	0.50
1:B:38:VAL:HG21	1:B:73:VAL:HG11	1.94	0.50
1:B:192:ILE:HG23	1:B:203:PHE:CE2	2.47	0.50
1:B:403:VAL:HG12	1:B:404:ALA:N	2.27	0.50
1:A:23:SER:HB3	1:A:121:SER:HB3	1.94	0.50
1:A:387:LEU:HD23	1:A:428:ILE:CD1	2.42	0.50
1:A:392:ARG:HB3	1:A:393:PRO:C	2.36	0.50
1:B:380:ASN:O	1:B:381:ASN:C	2.55	0.50
1:B:496:ILE:HG12	1:B:525:ILE:HD12	1.94	0.50
1:A:120:GLY:HA2	1:A:123:THR:CG2	2.40	0.49
1:A:481:ILE:O	1:A:485:ILE:HG23	2.12	0.49
1:A:628:ASN:HB3	1:A:631:CYS:HB3	1.94	0.49
1:B:280:LYS:HB2	1:B:293:VAL:HG21	1.93	0.49
1:B:289:TYR:O	1:B:291:THR:N	2.45	0.49
1:B:344:VAL:HG23	1:B:344:VAL:O	2.11	0.49
1:B:531:ASN:HD21	1:B:538:PHE:CA	2.25	0.49
1:B:421:SER:O	1:B:425:ILE:N	2.39	0.49
1:A:252:THR:C	1:A:254:GLY:H	2.20	0.49
1:A:295:VAL:HG12	1:A:295:VAL:O	2.10	0.49
1:A:371:MET:O	1:A:379:MET:HE2	2.12	0.49
1:B:741:TRP:CG	1:B:742:TRP:N	2.80	0.49
1:A:393:PRO:HB3	1:A:453:TRP:CE3	2.47	0.49
1:A:596:PHE:C	1:A:598:GLU:H	2.21	0.49
1:B:159:VAL:CG2	1:B:324:LEU:HD23	2.34	0.49
1:B:403:VAL:CG2	1:B:684:MET:HE1	2.42	0.49
1:B:508:LEU:O	1:B:509:MET:C	2.55	0.49
1:B:562:GLY:O	1:B:564:LYS:N	2.45	0.49
1:A:50:PHE:CZ	1:A:84:ILE:HD11	2.47	0.49
1:A:388:LEU:CD2	1:A:424:ARG:HB2	2.42	0.49
1:A:418:ALA:HB2	1:A:676:ALA:HB1	1.94	0.49
1:A:482:SER:HA	1:A:485:ILE:HG23	1.94	0.49
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.93	0.49
1:A:65:ILE:HB	1:A:108:ARG:HH12	1.78	0.49
1:A:125:ALA:O	1:A:128:PHE:HB3	2.13	0.49
1:B:69:THR:O	1:B:70:TRP:C	2.55	0.49
1:B:618:THR:CG2	1:B:619:THR:H	2.16	0.49
1:A:745:LEU:C	1:A:747:PRO:HD2	2.37	0.49
1:B:169:PHE:CZ	1:B:351:CYS:HB3	2.48	0.49
1:B:644:TYR:O	1:B:645:SER:C	2.54	0.49
1:A:70:TRP:CZ2	1:A:754:LYS:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:C	1:A:356:LYS:N	2.71	0.49
1:B:456:VAL:HA	1:B:459:TRP:CE2	2.48	0.49
1:A:169:PHE:CZ	1:A:351:CYS:HB3	2.48	0.49
1:A:714:ARG:HG3	1:A:719:VAL:HG13	1.95	0.49
1:A:742:TRP:C	1:A:744:LYS:N	2.69	0.49
1:B:352:VAL:O	1:B:355:THR:HB	2.12	0.49
1:A:66:ARG:NH2	1:A:108:ARG:NH2	2.61	0.48
1:A:336:VAL:HA	1:A:344:VAL:O	2.13	0.48
1:A:377:SER:O	1:A:378:PHE:C	2.55	0.48
1:B:185:ILE:C	1:B:185:ILE:HD13	2.37	0.48
1:B:279:VAL:C	1:B:281:ASP:N	2.70	0.48
1:A:367:PHE:O	1:A:370:ALA:HB3	2.14	0.48
1:B:283:VAL:CG2	1:B:284:VAL:H	2.26	0.48
1:B:360:LYS:O	1:B:363:ASP:N	2.44	0.48
1:B:416:ASN:O	1:B:417:ALA:C	2.55	0.48
1:B:180:SER:O	1:B:181:ALA:C	2.56	0.48
1:B:193:THR:CG2	1:B:194:THR:N	2.76	0.48
1:B:734:HIS:O	1:B:735:ARG:C	2.54	0.48
1:B:734:HIS:O	1:B:736:ILE:N	2.46	0.48
1:A:216:ALA:O	1:A:219:THR:HG22	2.14	0.48
1:A:407:ASN:HA	1:A:496:ILE:O	2.12	0.48
1:A:669:THR:HB	1:A:670:PRO:HD2	1.96	0.48
1:A:696:ARG:HH11	1:A:696:ARG:CG	2.21	0.48
1:B:78:GLN:H	1:B:78:GLN:CD	2.20	0.48
1:B:400:SER:HB2	1:B:431:ASN:HA	1.94	0.48
1:B:424:ARG:HD2	1:B:453:TRP:CZ2	2.48	0.48
1:B:510:GLU:HA	1:B:510:GLU:OE1	2.13	0.48
1:A:696:ARG:NH1	1:A:696:ARG:CG	2.76	0.48
1:B:69:THR:HG23	1:B:72:SER:CB	2.41	0.48
1:B:562:GLY:C	1:B:564:LYS:N	2.68	0.48
1:B:41:GLY:HA2	1:B:44:THR:HG22	1.94	0.48
1:B:247:LEU:CA	1:B:250:THR:HG22	2.43	0.48
1:A:73:VAL:HG12	1:A:76:MET:SD	2.53	0.48
1:A:82:THR:HG21	1:A:86:SER:CB	2.41	0.48
1:A:635:TYR:N	1:A:635:TYR:CD2	2.79	0.48
1:B:435:VAL:HG12	1:B:467:LEU:HD21	1.95	0.48
1:A:21:LEU:HD23	1:A:21:LEU:C	2.38	0.48
1:A:65:ILE:HB	1:A:108:ARG:NH1	2.29	0.48
1:A:239:TRP:O	1:A:242:HIS:HB3	2.14	0.48
1:A:304:THR:OG1	1:A:305:PRO:HD2	2.14	0.48
1:A:679:MET:CE	1:A:718:LEU:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LEU:HB2	1:B:51:VAL:HB	1.94	0.48
1:B:109:GLY:O	1:B:110:ILE:C	2.57	0.48
1:B:122:LEU:O	1:B:125:ALA:HB3	2.13	0.48
1:B:747:PRO:O	1:B:751:ILE:HG23	2.14	0.48
1:B:751:ILE:HD11	1:B:752:LEU:HD23	1.95	0.48
1:A:613:VAL:C	1:A:615:LYS:N	2.71	0.48
1:B:111:THR:O	1:B:156:LEU:HD12	2.13	0.48
1:B:307:ALA:H	1:B:547:ASN:ND2	2.10	0.48
1:B:376:ARG:HH21	1:B:376:ARG:CB	2.26	0.48
1:B:741:TRP:CD2	1:B:742:TRP:N	2.82	0.48
1:B:742:TRP:C	1:B:744:LYS:H	2.21	0.48
1:B:751:ILE:CD1	1:B:752:LEU:HD23	2.43	0.48
1:A:69:THR:O	1:A:72:SER:OG	2.30	0.48
1:A:282:LEU:HG	1:A:283:VAL:N	2.28	0.48
1:A:319:GLU:HG3	1:A:336:VAL:CG1	2.44	0.48
1:B:312:LEU:O	1:B:316:MET:HG2	2.14	0.48
1:B:450:GLU:HG3	1:B:451:ALA:N	2.24	0.48
1:B:547:ASN:O	1:B:550:CYS:N	2.47	0.48
1:B:165:ILE:HB	1:B:181:ALA:HB2	1.96	0.47
1:B:214:TYR:O	1:B:216:ALA:N	2.46	0.47
1:B:470:LYS:HE2	1:B:471:ARG:N	2.26	0.47
1:B:547:ASN:O	1:B:548:THR:C	2.57	0.47
1:A:49:PHE:CD1	1:A:110:ILE:CD1	2.97	0.47
1:A:360:LYS:C	1:A:362:MET:N	2.71	0.47
1:A:391:ILE:CD1	1:A:392:ARG:N	2.73	0.47
1:A:687:MET:HE1	1:A:691:ILE:HD11	1.95	0.47
1:B:116:ILE:HG12	1:B:161:LEU:HB3	1.95	0.47
1:B:295:VAL:O	1:B:296:LEU:C	2.54	0.47
1:B:510:GLU:C	1:B:512:ARG:N	2.72	0.47
1:A:42:ILE:O	1:A:45:GLY:N	2.47	0.47
1:A:104:ASN:O	1:A:108:ARG:HG2	2.13	0.47
1:A:391:ILE:O	1:A:392:ARG:O	2.32	0.47
1:B:84:ILE:N	1:B:84:ILE:CD1	2.78	0.47
1:B:205:LEU:CD2	1:B:294:THR:HB	2.42	0.47
1:A:275:THR:HG23	1:A:278:GLY:H	1.80	0.47
1:B:459:TRP:CE2	1:B:466:LYS:NZ	2.77	0.47
1:B:510:GLU:C	1:B:512:ARG:H	2.22	0.47
1:A:212:CYS:SG	1:A:214:TYR:HB2	2.54	0.47
1:A:570:ILE:HA	1:A:657:ASN:O	2.14	0.47
1:A:679:MET:C	1:A:681:ALA:N	2.72	0.47
1:A:742:TRP:CZ3	1:A:743:LEU:HG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:LEU:O	1:A:746:ARG:C	2.55	0.47
1:B:30:MET:O	1:B:34:VAL:HG23	2.14	0.47
1:B:360:LYS:O	1:B:362:MET:N	2.48	0.47
1:B:549:ILE:CD1	1:B:659:LEU:HD13	2.38	0.47
1:A:66:ARG:NH1	1:A:67:GLU:H	2.11	0.47
1:A:78:GLN:H	1:A:78:GLN:CD	2.16	0.47
1:A:120:GLY:O	1:A:121:SER:C	2.58	0.47
1:A:239:TRP:CH2	1:A:274:ILE:HD12	2.49	0.47
1:A:742:TRP:C	1:A:744:LYS:H	2.21	0.47
1:B:234:PRO:HG3	1:B:367:PHE:CE1	2.49	0.47
1:B:247:LEU:CD2	1:B:258:ASN:ND2	2.72	0.47
1:B:370:ALA:O	1:B:374:ARG:N	2.48	0.47
1:B:402:THR:CG2	1:B:491:GLN:HE21	2.28	0.47
1:B:477:SER:O	1:B:481:ILE:HG23	2.14	0.47
1:B:512:ARG:NH2	1:B:707:SER:HB2	2.27	0.47
1:A:76:MET:O	1:A:77:LEU:C	2.58	0.47
1:A:335:VAL:HG23	1:A:348:LEU:CG	2.39	0.47
1:A:435:VAL:CG1	1:A:467:LEU:CD2	2.93	0.47
1:A:457:GLY:HA2	4:A:767:PO4:O3	2.15	0.47
1:A:565:ARG:NH1	1:A:618:THR:O	2.47	0.47
1:A:573:MET:HE3	1:A:661:HIS:CD2	2.44	0.47
1:A:689:GLY:O	1:A:691:ILE:N	2.48	0.47
1:B:506:LEU:HD23	1:B:506:LEU:HA	1.72	0.47
1:B:11:THR:HG23	1:B:12:LEU:N	2.30	0.47
1:B:100:ARG:O	1:B:104:ASN:ND2	2.47	0.47
1:B:756:GLU:O	1:B:756:GLU:HG2	2.14	0.47
1:A:371:MET:HE1	1:A:382:TRP:CD1	2.50	0.47
1:A:571:GLU:HB3	1:A:658:VAL:HG22	1.97	0.47
1:B:27:ALA:O	1:B:30:MET:HG3	2.15	0.47
1:B:149:GLU:O	1:B:153:SER:HB3	2.15	0.47
1:B:610:GLU:O	1:B:614:GLN:HG2	2.15	0.47
1:A:193:THR:CG2	1:A:194:THR:N	2.78	0.46
1:A:248:SER:O	1:A:249:GLU:C	2.59	0.46
1:A:424:ARG:HD2	1:A:453:TRP:CE2	2.50	0.46
1:B:531:ASN:ND2	1:B:538:PHE:HA	2.28	0.46
1:B:595:ILE:HD11	1:B:598:GLU:HB3	1.97	0.46
1:A:473:LEU:HD22	1:A:474:PRO:HD2	1.97	0.46
1:A:509:MET:O	1:A:510:GLU:C	2.59	0.46
1:B:280:LYS:C	1:B:283:VAL:HG22	2.40	0.46
1:B:420:ARG:NH1	1:B:460:THR:HG21	2.30	0.46
1:B:484:ASN:C	1:B:486:THR:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:LEU:O	1:B:609:VAL:HG23	2.15	0.46
1:A:382:TRP:CE2	1:A:386:LYS:HD2	2.50	0.46
1:A:435:VAL:HG13	1:A:467:LEU:HD22	1.97	0.46
1:A:604:ASP:O	1:A:605:LEU:C	2.57	0.46
1:A:714:ARG:HG3	1:A:719:VAL:CG1	2.46	0.46
1:B:279:VAL:O	1:B:281:ASP:N	2.47	0.46
1:B:340:GLY:O	1:B:342:GLN:HG3	2.16	0.46
1:B:358:VAL:O	1:B:358:VAL:HG12	2.15	0.46
1:B:402:THR:HG21	1:B:489:ASN:HD22	1.81	0.46
1:A:35:ARG:CD	1:A:77:LEU:HD13	2.45	0.46
1:A:117:GLY:O	1:A:163:GLY:N	2.46	0.46
1:A:393:PRO:HB3	1:A:453:TRP:CZ3	2.50	0.46
1:B:279:VAL:O	1:B:283:VAL:HG13	2.16	0.46
1:B:308:PHE:CZ	1:B:312:LEU:HD22	2.51	0.46
1:B:560:ALA:O	1:B:622:ARG:NH2	2.47	0.46
1:B:566:ARG:CD	1:B:653:ASP:HB3	2.45	0.46
1:B:605:LEU:HD12	1:B:605:LEU:HA	1.75	0.46
1:B:660:GLY:O	1:B:662:MET:N	2.47	0.46
1:B:742:TRP:C	1:B:744:LYS:N	2.74	0.46
1:A:264:GLU:C	1:A:266:ALA:H	2.23	0.46
1:B:249:GLU:O	1:B:253:ARG:N	2.48	0.46
1:B:601:THR:O	1:B:604:ASP:N	2.42	0.46
1:A:628:ASN:O	1:A:630:LYS:N	2.49	0.46
1:A:719:VAL:HG22	1:A:721:GLN:HG2	1.98	0.46
1:B:277:GLU:O	1:B:280:LYS:HB3	2.16	0.46
1:B:323:ALA:HA	1:B:345:ARG:NH1	2.31	0.46
1:B:387:LEU:CD2	1:B:428:ILE:HG21	2.45	0.46
1:B:509:MET:CE	1:B:705:PRO:HA	2.45	0.46
1:B:658:VAL:O	1:B:658:VAL:CG1	2.54	0.46
2:B:763:ATP:O5'	2:B:763:ATP:H8	1.98	0.46
1:A:58:LEU:CD1	1:A:105:LEU:HD21	2.40	0.46
1:A:454:SER:O	1:A:455:TYR:C	2.59	0.46
1:B:302:GLY:O	1:B:303:GLY:O	2.33	0.46
1:B:387:LEU:HD23	1:B:428:ILE:HD13	1.98	0.46
1:B:459:TRP:CG	1:B:466:LYS:NZ	2.83	0.46
1:B:475:LYS:C	1:B:477:SER:H	2.23	0.46
1:B:512:ARG:HG2	1:B:519:CYS:SG	2.56	0.46
1:B:618:THR:CG2	1:B:619:THR:N	2.64	0.46
1:B:687:MET:HE1	1:B:691:ILE:CD1	2.45	0.46
1:A:243:LEU:CD1	1:A:247:LEU:HD12	2.46	0.46
1:A:544:THR:O	1:A:545:ALA:C	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:TYR:OH	1:A:608:ASN:ND2	2.46	0.46
1:A:597:GLU:H	1:A:597:GLU:CD	2.21	0.46
1:B:192:ILE:HG23	1:B:203:PHE:CZ	2.50	0.46
1:B:251:ARG:C	1:B:253:ARG:H	2.23	0.46
1:B:336:VAL:HG23	1:B:336:VAL:O	2.16	0.46
1:A:50:PHE:CD2	1:A:84:ILE:HD11	2.51	0.46
1:A:328:THR:C	1:A:330:ASP:N	2.73	0.46
1:A:673:ARG:O	1:A:677:THR:HB	2.15	0.46
1:B:342:GLN:NE2	1:B:715:LYS:HD2	2.31	0.46
1:A:165:ILE:N	1:A:165:ILE:CD1	2.79	0.46
1:A:566:ARG:H	1:A:616:MET:HE1	1.81	0.46
1:B:31:ASN:HB3	1:B:76:MET:HE2	1.99	0.46
1:B:621:LYS:O	1:B:622:ARG:HD2	2.16	0.46
1:B:565:ARG:HA	1:B:621:LYS:O	2.16	0.45
1:A:56:GLN:O	1:A:58:LEU:N	2.50	0.45
1:A:517:GLU:C	1:A:519:CYS:N	2.74	0.45
1:A:596:PHE:C	1:A:598:GLU:N	2.74	0.45
1:A:328:THR:O	1:A:330:ASP:N	2.49	0.45
1:B:124:GLY:C	1:B:127:THR:HG22	2.41	0.45
1:B:440:PHE:C	1:B:443:PRO:HD2	2.40	0.45
1:A:459:TRP:NE1	1:A:466:LYS:HZ3	2.13	0.45
1:B:184:ARG:HD3	1:B:187:GLU:OE2	2.16	0.45
1:B:609:VAL:HG22	1:B:644:TYR:CD2	2.48	0.45
1:A:12:LEU:HD23	1:A:325:LEU:HD13	1.98	0.45
1:A:42:ILE:O	1:A:44:THR:N	2.49	0.45
1:A:506:LEU:HD23	1:A:723:VAL:HB	1.98	0.45
1:A:556:ILE:O	1:A:558:GLN:N	2.45	0.45
1:A:748:ILE:HG12	1:A:749:LEU:H	1.82	0.45
1:B:299:VAL:O	1:B:302:GLY:N	2.37	0.45
1:A:606:GLN:OE1	1:B:606:GLN:OE1	2.35	0.45
1:B:404:ALA:HB2	1:B:490:ILE:CD1	2.46	0.45
1:B:748:ILE:O	1:B:752:LEU:HG	2.16	0.45
1:A:21:LEU:HD23	1:A:22:THR:N	2.32	0.45
1:A:339:SER:OG	1:A:344:VAL:HG11	2.16	0.45
1:A:109:GLY:C	1:A:110:ILE:HG12	2.41	0.45
1:A:153:SER:C	1:A:155:TYR:N	2.70	0.45
1:A:227:TRP:CD1	1:A:228:VAL:H	2.34	0.45
1:A:280:LYS:HB2	1:A:293:VAL:CG2	2.47	0.45
1:A:564:LYS:O	1:A:565:ARG:O	2.35	0.45
1:A:690:LYS:HE3	1:A:706:ASP:HB2	1.98	0.45
1:B:376:ARG:HB3	1:B:376:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLY:HA3	1:A:540:VAL:CG1	2.46	0.45
1:B:11:THR:C	1:B:13:GLY:N	2.75	0.45
1:B:376:ARG:NH2	1:B:376:ARG:HB2	2.32	0.45
1:B:459:TRP:HD1	1:B:459:TRP:N	2.05	0.45
1:B:502:TYR:OH	1:B:730:THR:CG2	2.64	0.45
1:B:552:THR:HG21	1:B:659:LEU:CD2	2.47	0.45
1:A:413:ALA:HB1	1:A:668:PRO:HA	1.98	0.45
1:B:340:GLY:O	1:B:342:GLN:N	2.51	0.45
1:B:638:ASP:OD1	1:B:638:ASP:N	2.49	0.45
1:A:203:PHE:CD1	1:A:203:PHE:N	2.85	0.44
1:A:391:ILE:CD1	2:A:765:ATP:PG	3.02	0.44
1:A:486:THR:HG22	1:A:487:LYS:N	2.32	0.44
1:A:502:TYR:OH	1:A:730:THR:HG21	2.17	0.44
1:A:652:PHE:HD1	1:A:653:ASP:O	1.99	0.44
1:B:83:VAL:HG12	1:B:84:ILE:HD12	1.99	0.44
1:B:484:ASN:O	1:B:485:ILE:C	2.60	0.44
1:B:548:THR:O	1:B:549:ILE:C	2.60	0.44
1:B:551:THR:HG22	1:B:552:THR:H	1.80	0.44
1:A:319:GLU:HG3	1:A:336:VAL:HB	1.99	0.44
1:A:398:SER:C	1:A:400:SER:N	2.75	0.44
1:A:571:GLU:HA	1:A:627:ARG:O	2.17	0.44
1:B:193:THR:C	1:B:195:THR:N	2.75	0.44
1:B:333:ALA:HB3	1:B:348:LEU:HB2	1.99	0.44
1:B:696:ARG:HB3	1:B:697:ASN:H	1.51	0.44
1:A:168:ASP:O	1:A:169:PHE:C	2.58	0.44
1:A:407:ASN:HB3	1:A:469:SER:HB3	1.99	0.44
1:B:433:VAL:O	1:B:434:LEU:HD12	2.17	0.44
1:B:459:TRP:O	1:B:460:THR:C	2.59	0.44
1:B:659:LEU:HD23	1:B:659:LEU:HA	1.73	0.44
1:A:159:VAL:HG11	1:A:320:ALA:HA	1.99	0.44
1:A:711:LEU:CD1	1:A:718:LEU:HG	2.46	0.44
1:B:403:VAL:HG21	1:B:684:MET:CE	2.46	0.44
1:B:509:MET:HE1	1:B:705:PRO:HA	1.99	0.44
1:A:13:GLY:O	1:A:46:ALA:HA	2.17	0.44
1:A:537:ASP:OD1	1:A:714:ARG:NH2	2.37	0.44
1:B:190:ASP:O	1:B:193:THR:HG22	2.17	0.44
1:B:215:LEU:O	1:B:219:THR:HG21	2.16	0.44
1:A:629:GLU:O	1:A:630:LYS:HG3	2.17	0.44
1:B:84:ILE:O	1:B:84:ILE:HG22	2.17	0.44
1:B:367:PHE:C	1:B:369:GLU:N	2.75	0.44
1:A:165:ILE:HD13	1:A:165:ILE:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:TRP:NE1	1:A:466:LYS:NZ	2.65	0.44
1:A:742:TRP:CE3	1:A:743:LEU:HG	2.53	0.44
1:B:11:THR:C	1:B:13:GLY:H	2.26	0.44
1:B:485:ILE:C	1:B:485:ILE:CD1	2.90	0.44
1:A:174:MET:HE2	3:A:764:ADP:C8	2.53	0.44
1:A:294:THR:CG2	1:A:295:VAL:N	2.81	0.44
1:A:524:VAL:HB	1:A:710:VAL:CG2	2.47	0.44
1:A:582:THR:OG1	1:A:746:ARG:NH1	2.50	0.44
1:B:56:GLN:O	1:B:60:ASP:OD2	2.36	0.44
1:A:41:GLY:O	1:A:44:THR:HG22	2.17	0.44
1:A:408:VAL:O	1:A:497:GLY:CA	2.66	0.44
1:A:579:TYR:HD1	1:A:742:TRP:CD1	2.36	0.44
1:B:245:ARG:HH11	1:B:245:ARG:HG2	1.83	0.44
1:B:279:VAL:C	1:B:281:ASP:H	2.25	0.44
1:B:696:ARG:O	1:B:698:GLY:N	2.50	0.44
1:B:730:THR:O	1:B:738:LYS:HD2	2.17	0.44
1:B:754:LYS:O	1:B:755:TYR:O	2.36	0.44
1:A:689:GLY:O	1:A:690:LYS:C	2.60	0.43
1:A:140:GLN:NE2	1:A:144:LYS:O	2.51	0.43
1:A:232:GLU:OE2	1:A:374:ARG:NE	2.51	0.43
1:A:435:VAL:CG1	1:A:467:LEU:HD22	2.48	0.43
1:A:628:ASN:C	1:A:630:LYS:H	2.26	0.43
1:B:404:ALA:CB	1:B:490:ILE:HD12	2.47	0.43
1:B:555:ARG:HG2	1:B:556:ILE:N	2.34	0.43
1:A:53:GLU:O	1:A:54:GLY:C	2.62	0.43
1:A:598:GLU:HA	1:A:599:PRO:HD2	1.83	0.43
1:B:205:LEU:HB2	1:B:261:ILE:HD13	2.00	0.43
1:B:352:VAL:HA	1:B:355:THR:HB	1.99	0.43
1:B:393:PRO:HD3	1:B:453:TRP:CD2	2.53	0.43
1:B:658:VAL:O	1:B:659:LEU:C	2.59	0.43
1:A:239:TRP:CG	1:A:240:GLU:N	2.86	0.43
1:A:387:LEU:CD2	1:A:428:ILE:HD13	2.45	0.43
1:A:413:ALA:HB1	1:A:668:PRO:CA	2.49	0.43
1:B:193:THR:HA	1:B:257:LEU:HD11	2.00	0.43
1:A:257:LEU:HD23	1:A:257:LEU:N	2.20	0.43
1:A:358:VAL:HG22	1:A:373:LEU:HB3	2.00	0.43
1:A:509:MET:O	1:A:512:ARG:N	2.50	0.43
1:B:240:GLU:CG	1:B:282:LEU:HD22	2.49	0.43
1:B:244:CYS:C	1:B:246:ARG:N	2.74	0.43
1:B:307:ALA:O	1:B:311:ILE:HG12	2.18	0.43
1:B:481:ILE:HD12	1:B:485:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:THR:HG23	1:B:528:THR:O	2.19	0.43
1:B:576:TYR:CE1	1:B:630:LYS:HD2	2.53	0.43
1:A:186:THR:HG22	1:A:190:ASP:OD2	2.18	0.43
1:A:522:PHE:C	1:A:522:PHE:CD2	2.96	0.43
1:A:686:TRP:HZ3	1:A:687:MET:HG2	1.82	0.43
1:B:98:ARG:O	1:B:99:LEU:C	2.60	0.43
1:B:243:LEU:HD12	1:B:243:LEU:O	2.17	0.43
1:B:424:ARG:HD2	1:B:453:TRP:CH2	2.54	0.43
1:B:485:ILE:CG1	1:B:517:GLU:HB3	2.48	0.43
1:B:609:VAL:HG22	1:B:644:TYR:CZ	2.50	0.43
1:A:679:MET:HG2	1:A:718:LEU:HD21	2.01	0.43
1:A:38:VAL:O	1:A:42:ILE:HG12	2.19	0.43
1:A:185:ILE:CD1	1:A:215:LEU:HD23	2.49	0.43
1:B:193:THR:O	1:B:195:THR:N	2.52	0.43
1:B:355:THR:HG22	1:B:356:LYS:N	2.34	0.43
1:B:370:ALA:O	1:B:371:MET:C	2.60	0.43
1:B:566:ARG:HD2	1:B:653:ASP:OD2	2.18	0.43
1:B:615:LYS:HB3	1:B:620:VAL:CG2	2.48	0.43
1:B:687:MET:HE1	1:B:691:ILE:CG1	2.48	0.43
1:A:13:GLY:CA	1:A:44:THR:O	2.66	0.43
1:A:50:PHE:C	1:A:51:VAL:HG23	2.44	0.43
1:A:258:ASN:O	1:A:259:ILE:HD12	2.18	0.43
1:A:459:TRP:O	1:A:460:THR:C	2.62	0.43
1:A:558:GLN:O	1:A:559:SER:O	2.37	0.43
1:B:55:TYR:O	1:B:56:GLN:C	2.62	0.43
1:B:384:VAL:O	1:B:385:TYR:C	2.62	0.43
1:B:414:GLY:HA3	1:B:540:VAL:CG1	2.49	0.43
1:A:59:VAL:O	1:A:60:ASP:C	2.62	0.43
1:A:544:THR:OG1	1:A:669:THR:HG23	2.19	0.43
1:A:684:MET:O	1:A:684:MET:HG3	2.19	0.43
1:B:78:GLN:OE1	1:B:78:GLN:N	2.37	0.43
1:B:113:LEU:O	1:B:158:ILE:HA	2.19	0.43
1:A:252:THR:C	1:A:254:GLY:N	2.77	0.42
1:A:275:THR:HG23	1:A:278:GLY:N	2.34	0.42
1:B:200:GLN:HA	1:B:256:ARG:O	2.19	0.42
1:B:377:SER:O	1:B:378:PHE:C	2.62	0.42
1:B:379:MET:HE3	1:B:379:MET:HB2	1.79	0.42
1:B:382:TRP:O	1:B:383:GLU:C	2.62	0.42
1:B:402:THR:CG2	1:B:432:ARG:HH21	2.30	0.42
1:B:520:ILE:HA	1:B:521:PRO:HD3	1.84	0.42
1:A:191:ALA:O	1:A:192:ILE:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PRO:HG3	1:A:367:PHE:CZ	2.53	0.42
1:A:564:LYS:HE2	1:A:564:LYS:CA	2.50	0.42
1:B:208:MET:HE3	1:B:300:GLN:OE1	2.19	0.42
1:B:242:HIS:O	1:B:246:ARG:HG2	2.19	0.42
1:A:112:ASN:HB3	1:A:324:LEU:HD13	2.01	0.42
1:A:307:ALA:O	1:A:311:ILE:HG13	2.19	0.42
1:A:634:ASN:HB2	1:B:646:GLU:CG	2.48	0.42
1:A:669:THR:CB	1:A:670:PRO:HD2	2.49	0.42
1:B:218:VAL:HG12	1:B:219:THR:N	2.35	0.42
1:B:328:THR:CB	1:B:329:PRO:CD	2.93	0.42
1:A:158:ILE:HD13	1:A:158:ILE:H	1.84	0.42
1:A:319:GLU:CG	1:A:336:VAL:HB	2.50	0.42
1:A:429:GLN:HE22	1:A:685:ASN:HA	1.85	0.42
1:A:564:LYS:HB3	1:A:565:ARG:H	1.72	0.42
1:A:604:ASP:O	1:A:606:GLN:N	2.52	0.42
1:B:190:ASP:C	1:B:193:THR:HG22	2.44	0.42
1:B:319:GLU:HG3	1:B:336:VAL:HB	2.01	0.42
1:B:359:THR:O	1:B:362:MET:HB2	2.19	0.42
1:B:549:ILE:HD12	1:B:659:LEU:CD1	2.37	0.42
1:A:227:TRP:HB3	1:A:260:ILE:HG23	2.00	0.42
1:A:529:VAL:HG11	1:A:573:MET:HE2	2.01	0.42
1:B:29:GLY:HA3	1:B:176:ILE:CG2	2.49	0.42
1:B:185:ILE:CD1	1:B:219:THR:HB	2.49	0.42
1:B:554:ASP:O	1:B:557:LYS:HB3	2.19	0.42
1:A:65:ILE:HG22	1:A:65:ILE:O	2.19	0.42
1:A:388:LEU:HD23	1:A:424:ARG:CB	2.49	0.42
1:A:491:GLN:CB	1:A:700:ILE:HD11	2.39	0.42
1:B:284:VAL:HA	1:B:288:GLY:HA2	2.02	0.42
1:A:33:ALA:O	1:A:34:VAL:C	2.60	0.42
1:A:193:THR:CG2	1:A:194:THR:HG23	2.50	0.42
1:A:352:VAL:O	1:A:355:THR:HG22	2.20	0.42
1:A:566:ARG:N	1:A:616:MET:HE1	2.34	0.42
1:A:751:ILE:HD11	1:A:752:LEU:HD23	2.02	0.42
1:B:132:TRP:CE3	1:B:156:LEU:HD22	2.55	0.42
1:B:192:ILE:HD13	1:B:192:ILE:N	2.34	0.42
1:B:237:ASP:C	1:B:239:TRP:N	2.77	0.42
1:B:240:GLU:HG2	1:B:282:LEU:HD22	2.02	0.42
1:B:481:ILE:HD12	1:B:485:ILE:CG2	2.50	0.42
1:A:13:GLY:N	1:A:44:THR:O	2.53	0.42
1:A:18:ILE:CG2	1:A:112:ASN:HB2	2.41	0.42
1:A:360:LYS:O	1:A:362:MET:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLN:H	1:A:480:GLN:CD	2.27	0.42
1:A:575:GLY:HA2	1:A:630:LYS:HE2	2.02	0.42
1:B:204:VAL:HB	1:B:293:VAL:HG22	2.01	0.42
1:B:502:TYR:O	1:B:505:GLY:N	2.42	0.42
1:B:509:MET:O	1:B:510:GLU:C	2.61	0.42
1:B:679:MET:HE2	1:B:679:MET:HA	2.02	0.42
1:A:261:ILE:HD12	1:A:261:ILE:N	2.35	0.42
1:B:110:ILE:HD12	1:B:110:ILE:N	2.33	0.42
1:B:342:GLN:HE21	1:B:715:LYS:HD2	1.84	0.42
1:B:628:ASN:HB3	1:B:631:CYS:HB3	2.01	0.42
1:A:193:THR:HG23	1:A:194:THR:HG23	2.01	0.42
1:A:344:VAL:HG23	1:A:346:LEU:HG	2.01	0.42
1:A:506:LEU:HD21	1:A:723:VAL:C	2.44	0.42
1:A:565:ARG:HH21	1:A:565:ARG:CG	2.32	0.42
1:B:84:ILE:O	1:B:84:ILE:CG2	2.68	0.42
1:B:184:ARG:HA	1:B:184:ARG:HD3	1.76	0.42
1:B:228:VAL:HG23	1:B:385:TYR:CE2	2.55	0.42
1:A:92:PHE:C	1:A:94:GLU:H	2.27	0.41
1:A:138:ASP:C	1:A:140:GLN:N	2.78	0.41
1:A:323:ALA:HA	1:A:345:ARG:NH1	2.35	0.41
1:A:500:GLU:CD	1:A:735:ARG:NH2	2.78	0.41
1:A:549:ILE:O	1:A:550:CYS:C	2.64	0.41
1:A:634:ASN:HB2	1:B:646:GLU:HG2	2.02	0.41
1:A:158:ILE:HD13	1:A:158:ILE:O	2.20	0.41
1:A:326:GLU:CD	1:A:345:ARG:HH22	2.28	0.41
1:A:377:SER:O	1:A:380:ASN:N	2.53	0.41
1:A:524:VAL:HB	1:A:710:VAL:HG22	2.02	0.41
1:B:280:LYS:HB2	1:B:293:VAL:CG2	2.50	0.41
1:B:585:GLY:CA	1:B:626:LEU:HD12	2.47	0.41
1:B:649:LYS:C	1:B:651:ILE:N	2.77	0.41
1:A:39:ARG:CD	1:A:70:TRP:CE2	3.02	0.41
1:A:370:ALA:C	1:A:372:LYS:N	2.78	0.41
1:B:41:GLY:CA	1:B:44:THR:HG22	2.49	0.41
1:B:69:THR:O	1:B:72:SER:N	2.41	0.41
1:B:244:CYS:O	1:B:245:ARG:C	2.64	0.41
1:B:645:SER:O	1:B:646:GLU:C	2.62	0.41
1:A:22:THR:HG23	1:A:85:GLY:O	2.21	0.41
1:A:290:ASP:O	1:A:290:ASP:CG	2.63	0.41
1:A:601:THR:O	1:A:602:ILE:C	2.61	0.41
1:B:59:VAL:HA	1:B:101:ALA:HB2	2.03	0.41
1:B:103:HIS:O	1:B:104:ASN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:TRP:CD2	1:B:156:LEU:HD22	2.56	0.41
1:A:505:GLY:O	1:A:508:LEU:N	2.42	0.41
1:A:506:LEU:O	1:A:507:GLU:C	2.62	0.41
1:A:618:THR:HG22	1:A:619:THR:N	2.35	0.41
1:B:131:GLU:C	1:B:135:LEU:HD12	2.45	0.41
1:B:237:ASP:C	1:B:239:TRP:H	2.28	0.41
1:B:489:ASN:CG	1:B:489:ASN:O	2.63	0.41
1:B:578:GLY:HA3	1:B:595:ILE:HB	2.02	0.41
1:B:627:ARG:HG2	1:B:627:ARG:HH11	1.85	0.41
1:A:50:PHE:O	1:A:51:VAL:CG2	2.67	0.41
1:A:169:PHE:CE2	1:A:351:CYS:HB3	2.56	0.41
1:A:435:VAL:CG1	1:A:467:LEU:HD21	2.51	0.41
1:A:581:ALA:O	1:A:585:GLY:N	2.50	0.41
1:A:609:VAL:HG22	1:A:644:TYR:CZ	2.55	0.41
1:B:63:ASP:O	1:B:65:ILE:N	2.53	0.41
1:B:101:ALA:O	1:B:104:ASN:HB2	2.21	0.41
1:B:181:ALA:O	1:B:185:ILE:HG22	2.21	0.41
1:B:520:ILE:CG2	1:B:700:ILE:HD11	2.40	0.41
1:A:515:PHE:CD1	1:A:515:PHE:N	2.89	0.41
1:B:193:THR:HA	1:B:257:LEU:CD1	2.50	0.41
1:B:251:ARG:C	1:B:253:ARG:N	2.75	0.41
1:B:402:THR:HB	1:B:432:ARG:HE	1.85	0.41
1:B:551:THR:CG2	1:B:552:THR:N	2.78	0.41
1:A:162:VAL:CG1	1:A:175:THR:HG22	2.50	0.41
1:A:215:LEU:O	1:A:219:THR:HB	2.21	0.41
1:A:473:LEU:HA	1:A:473:LEU:HD23	1.63	0.41
1:A:586:LEU:HD12	1:A:586:LEU:C	2.46	0.41
1:B:419:VAL:CG1	1:B:467:LEU:HD11	2.43	0.41
1:B:524:VAL:HB	1:B:710:VAL:HG22	2.02	0.41
1:B:632:ASN:OD1	1:B:634:ASN:N	2.54	0.41
1:A:181:ALA:O	1:A:185:ILE:HG13	2.21	0.41
1:A:247:LEU:HD11	1:A:260:ILE:HD11	2.03	0.41
1:A:491:GLN:HE21	1:A:700:ILE:HD13	1.86	0.41
1:A:628:ASN:C	1:A:628:ASN:OD1	2.64	0.41
1:B:22:THR:HG21	1:B:82:THR:OG1	2.20	0.41
1:B:39:ARG:HG3	1:B:39:ARG:NH1	2.33	0.41
1:B:299:VAL:CG2	1:B:300:GLN:N	2.84	0.41
1:B:359:THR:O	1:B:360:LYS:C	2.64	0.41
1:B:423:VAL:HG12	1:B:427:LEU:HD11	2.02	0.41
1:A:388:LEU:HD23	1:A:424:ARG:HB2	2.02	0.41
1:A:604:ASP:C	1:A:606:GLN:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:SER:O	1:B:154:SER:C	2.64	0.41
1:B:230:ILE:HA	1:B:231:PRO:HD3	1.87	0.41
1:B:471:ARG:NH2	4:B:768:PO4:O1	2.53	0.41
1:A:403:VAL:CG1	1:A:404:ALA:N	2.84	0.40
1:A:414:GLY:HA3	1:A:540:VAL:HG11	2.03	0.40
1:A:493:LEU:O	1:A:522:PHE:HA	2.21	0.40
1:B:229:PHE:HZ	1:B:239:TRP:CZ3	2.39	0.40
1:A:101:ALA:O	1:A:104:ASN:HB2	2.22	0.40
1:A:184:ARG:HD2	1:A:302:GLY:O	2.21	0.40
1:A:208:MET:CG	1:A:209:GLY:H	2.33	0.40
1:A:214:TYR:O	1:A:215:LEU:C	2.64	0.40
1:A:473:LEU:HB3	1:A:474:PRO:HD2	2.03	0.40
1:A:602:ILE:O	1:A:602:ILE:HG13	2.21	0.40
1:A:681:ALA:O	1:A:682:LYS:C	2.63	0.40
1:B:723:VAL:HG23	1:B:724:THR:H	1.86	0.40
1:A:473:LEU:HD22	1:A:504:GLY:HA2	2.02	0.40
1:A:689:GLY:C	1:A:691:ILE:N	2.78	0.40
1:B:377:SER:O	1:B:380:ASN:N	2.52	0.40
1:B:386:LYS:HB3	1:B:386:LYS:HE2	1.94	0.40
1:B:649:LYS:HD2	1:B:649:LYS:HA	1.88	0.40
1:B:727:GLN:C	1:B:729:GLN:N	2.77	0.40
1:A:186:THR:O	1:A:190:ASP:HB2	2.21	0.40
1:A:632:ASN:OD1	1:A:632:ASN:C	2.65	0.40
1:B:145:ILE:C	1:B:147:ALA:N	2.78	0.40
1:B:235:PRO:HB2	1:B:239:TRP:CB	2.52	0.40
1:B:604:ASP:O	1:B:605:LEU:C	2.64	0.40
1:A:56:GLN:O	1:A:57:GLY:C	2.63	0.40
1:A:173:ASP:HB3	3:A:764:ADP:H4'	2.02	0.40
1:A:447:GLN:C	1:A:448:ILE:HG13	2.46	0.40
1:B:403:VAL:HG12	1:B:404:ALA:H	1.85	0.40
1:B:440:PHE:C	1:B:442:GLY:N	2.78	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	746/762 (98%)	564 (76%)	123 (16%)	59 (8%)	1	5
1	B	746/762 (98%)	565 (76%)	119 (16%)	62 (8%)	0	4
All	All	1492/1524 (98%)	1129 (76%)	242 (16%)	121 (8%)	1	4

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PHE
1	A	51	VAL
1	A	54	GLY
1	A	60	ASP
1	A	153	SER
1	A	198	SER
1	A	214	TYR
1	A	238	ASN
1	A	297	GLY
1	A	298	HIS
1	A	365	LYS
1	A	375	GLY
1	A	392	ARG
1	A	559	SER
1	A	565	ARG
1	B	60	ASP
1	B	62	GLY
1	B	232	GLU
1	B	291	THR
1	B	303	GLY
1	B	390	HIS
1	B	445	LYS
1	B	466	LYS
1	B	602	ILE
1	B	645	SER
1	B	664	GLN
1	B	735	ARG
1	B	753	ALA
1	A	56	GLN
1	A	57	GLY
1	A	142	ALA
1	A	143	GLY
1	A	152	ARG

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Mol	Chain	Res	Type
1	A	154	SER
1	A	196	ALA
1	A	236	ASP
1	A	476	LYS
1	A	564	LYS
1	A	629	GLU
1	A	647	GLU
1	A	663	GLN
1	A	666	GLY
1	A	680	GLY
1	A	690	LYS
1	B	12	LEU
1	B	64	HIS
1	B	107	LYS
1	B	110	ILE
1	B	154	SER
1	B	194	THR
1	B	201	ARG
1	B	208	MET
1	B	237	ASP
1	B	247	LEU
1	B	280	LYS
1	B	282	LEU
1	B	290	ASP
1	B	332	PRO
1	B	341	ASN
1	B	361	ALA
1	B	365	LYS
1	B	397	LYS
1	B	465	SER
1	B	476	LYS
1	B	511	GLY
1	B	551	THR
1	B	563	THR
1	B	565	ARG
1	B	589	GLY
1	B	597	GLU
1	B	618	THR
1	B	661	HIS
1	B	666	GLY
1	B	755	TYR
1	A	126	ASP

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Mol	Chain	Res	Type
1	A	208	MET
1	A	235	PRO
1	A	272	LYS
1	A	273	PRO
1	A	296	LEU
1	A	390	HIS
1	A	560	ALA
1	A	597	GLU
1	A	602	ILE
1	A	605	LEU
1	A	645	SER
1	B	16	LYS
1	B	75	MET
1	B	141	LYS
1	B	146	THR
1	B	555	ARG
1	B	559	SER
1	B	564	LYS
1	B	662	MET
1	A	28	GLN
1	A	109	GLY
1	A	131	GLU
1	A	619	THR
1	A	646	GLU
1	B	198	SER
1	B	215	LEU
1	B	382	TRP
1	B	510	GLU
1	B	697	ASN
1	A	200	GLN
1	A	371	MET
1	A	580	LEU
1	A	618	THR
1	A	641	PHE
1	A	662	MET
1	A	693	GLU
1	B	199	HIS
1	B	396	PRO
1	B	561	ALA
1	B	579	TYR
1	A	201	ARG
1	B	446	GLY

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Mol	Chain	Res	Type
1	A	42	ILE
1	B	698	GLY
1	A	62	GLY
1	A	329	PRO

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	605/618 (98%)	525 (87%)	80 (13%)	4	19
1	B	605/618 (98%)	527 (87%)	78 (13%)	4	20
All	All	1210/1236 (98%)	1052 (87%)	158 (13%)	4	19

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	22	THR
1	A	28	GLN
1	A	66	ARG
1	A	73	VAL
1	A	77	LEU
1	A	78	GLN
1	A	84	ILE
1	A	106	VAL
1	A	126	ASP
1	A	127	THR
1	A	140	GLN
1	A	155	TYR
1	A	158	ILE
1	A	164	SER
1	A	165	ILE
1	A	178	THR
1	A	180	SER
1	A	190	ASP

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Mol	Chain	Res	Type
1	A	192	ILE
1	A	193	THR
1	A	200	GLN
1	A	222	SER
1	A	226	ASP
1	A	243	LEU
1	A	257	LEU
1	A	275	THR
1	A	276	SER
1	A	277	GLU
1	A	299	VAL
1	A	304	THR
1	A	314	SER
1	A	336	VAL
1	A	344	VAL
1	A	348	LEU
1	A	352	VAL
1	A	387	LEU
1	A	391	ILE
1	A	402	THR
1	A	405	VAL
1	A	428	ILE
1	A	435	VAL
1	A	460	THR
1	A	462	GLN
1	A	481	ILE
1	A	485	ILE
1	A	486	THR
1	A	493	LEU
1	A	495	ILE
1	A	500	GLU
1	A	503	THR
1	A	507	GLU
1	A	516	ASP
1	A	523	VAL
1	A	529	VAL
1	A	544	THR
1	A	547	ASN
1	A	551	THR
1	A	552	THR
1	A	553	CYS
1	A	564	LYS

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Mol	Chain	Res	Type
1	A	566	ARG
1	A	614	GLN
1	A	657	ASN
1	A	669	THR
1	A	674	ASN
1	A	677	THR
1	A	685	ASN
1	A	687	MET
1	A	693	GLU
1	A	700	ILE
1	A	706	ASP
1	A	710	VAL
1	A	714	ARG
1	A	719	VAL
1	A	730	THR
1	A	731	ASP
1	A	740	GLN
1	A	748	ILE
1	A	751	ILE
1	B	18	ILE
1	B	21	LEU
1	B	22	THR
1	B	26	ASP
1	B	69	THR
1	B	78	GLN
1	B	83	VAL
1	B	89	CYS
1	B	129	ARG
1	B	158	ILE
1	B	165	ILE
1	B	173	ASP
1	B	178	THR
1	B	185	ILE
1	B	186	THR
1	B	189	VAL
1	B	192	ILE
1	B	200	GLN
1	B	208	MET
1	B	210	ARG
1	B	219	THR
1	B	238	ASN
1	B	274	ILE

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Mol	Chain	Res	Type
1	B	275	THR
1	B	318	VAL
1	B	348	LEU
1	B	355	THR
1	B	368	ASP
1	B	373	LEU
1	B	374	ARG
1	B	402	THR
1	B	405	VAL
1	B	406	MET
1	B	411	PRO
1	B	420	ARG
1	B	435	VAL
1	B	450	GLU
1	B	454	SER
1	B	460	THR
1	B	462	GLN
1	B	466	LYS
1	B	467	LEU
1	B	470	LYS
1	B	481	ILE
1	B	485	ILE
1	B	493	LEU
1	B	500	GLU
1	B	503	THR
1	B	509	MET
1	B	514	GLN
1	B	517	GLU
1	B	530	SER
1	B	550	CYS
1	B	551	THR
1	B	553	CYS
1	B	566	ARG
1	B	573	MET
1	B	582	THR
1	B	595	ILE
1	B	632	ASN
1	B	642	ASN
1	B	658	VAL
1	B	679	MET
1	B	687	MET
1	B	703	ASN

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Mol	Chain	Res	Type
1	B	707	SER
1	B	713	MET
1	B	714	ARG
1	B	719	VAL
1	B	723	VAL
1	B	724	THR
1	B	730	THR
1	B	731	ASP
1	B	733	GLU
1	B	743	LEU
1	B	749	LEU
1	B	751	ILE
1	B	754	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	64	HIS
1	A	104	ASN
1	A	157	ASN
1	A	298	HIS
1	A	380	ASN
1	A	429	GLN
1	A	431	ASN
1	A	437	HIS
1	A	447	GLN
1	A	462	GLN
1	A	491	GLN
1	A	514	GLN
1	A	531	ASN
1	A	608	ASN
1	A	611	HIS
1	A	634	ASN
1	A	642	ASN
1	A	661	HIS
1	A	674	ASN
1	A	703	ASN
1	A	734	HIS
1	A	740	GLN
1	B	104	ASN
1	B	183	HIS

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Mol	Chain	Res	Type
1	B	242	HIS
1	B	258	ASN
1	B	342	GLN
1	B	407	ASN
1	B	431	ASN
1	B	437	HIS
1	B	480	GLN
1	B	489	ASN
1	B	491	GLN
1	B	514	GLN
1	B	531	ASN
1	B	547	ASN
1	B	611	HIS
1	B	634	ASN
1	B	642	ASN
1	B	674	ASN
1	B	703	ASN
1	B	727	GLN
1	B	734	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 ⓘ

12 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	$\# Z > 2$
2	ATP	B	763	-	32,33,33	1.16	3 (9%)	48,52,52	1.61	9 (18%)
4	PO4	B	767	-	4,4,4	2.01	3 (75%)	6,6,6	1.24	1 (16%)
4	PO4	A	768	-	4,4,4	1.99	3 (75%)	6,6,6	1.40	1 (16%)
4	PO4	A	767	-	4,4,4	1.99	3 (75%)	6,6,6	1.45	2 (33%)
2	ATP	A	763	-	32,33,33	1.21	3 (9%)	48,52,52	1.63	10 (20%)
2	ATP	A	765	-	32,33,33	1.19	3 (9%)	48,52,52	2.19	20 (41%)
3	ADP	B	764	-	28,29,29	1.15	3 (10%)	43,45,45	1.72	8 (18%)
4	PO4	B	768	-	4,4,4	2.00	3 (75%)	6,6,6	1.23	1 (16%)
4	PO4	B	766	-	4,4,4	2.04	3 (75%)	6,6,6	1.29	2 (33%)
3	ADP	A	764	-	28,29,29	1.16	3 (10%)	43,45,45	2.05	14 (32%)
2	ATP	B	765	-	32,33,33	1.15	3 (9%)	48,52,52	1.96	16 (33%)
4	PO4	A	766	-	4,4,4	2.01	3 (75%)	6,6,6	1.37	1 (16%)

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
2	ATP	B	763	-	-	4/22/38/38	0/3/3/3
2	ATP	A	763	-	-	4/22/38/38	0/3/3/3
2	ATP	A	765	-	-	5/22/38/38	0/3/3/3
3	ADP	B	764	-	-	2/16/32/32	0/3/3/3
3	ADP	A	764	-	-	2/16/32/32	0/3/3/3
2	ATP	B	765	-	-	4/22/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	765	ATP	C5-N7	-3.16	1.33	1.39
3	A	764	ADP	C5-N7	-3.15	1.33	1.39
2	A	765	ATP	C5-N7	-3.15	1.33	1.39
3	B	764	ADP	C5-N7	-3.13	1.33	1.39
2	A	763	ATP	C5-N7	-3.09	1.33	1.39
2	B	763	ATP	C5-N7	-3.06	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	765	ATP	C8-N9	-2.40	1.33	1.37
2	A	765	ATP	C8-N9	-2.38	1.33	1.37
4	B	766	PO4	P-O2	2.37	1.61	1.54
2	A	763	ATP	C8-N9	-2.37	1.33	1.37
4	B	766	PO4	P-O3	2.36	1.61	1.54
2	B	763	ATP	C8-N9	-2.36	1.33	1.37
4	A	766	PO4	P-O3	2.35	1.61	1.54
3	A	764	ADP	C8-N9	-2.35	1.33	1.37
4	A	768	PO4	P-O3	2.34	1.61	1.54
4	A	766	PO4	P-O2	2.32	1.61	1.54
4	B	767	PO4	P-O2	2.31	1.61	1.54
4	B	767	PO4	P-O3	2.29	1.61	1.54
4	B	768	PO4	P-O2	2.29	1.61	1.54
4	A	767	PO4	P-O3	2.29	1.61	1.54
3	B	764	ADP	C8-N9	-2.28	1.33	1.37
4	A	767	PO4	P-O2	2.28	1.61	1.54
4	B	768	PO4	P-O3	2.26	1.61	1.54
4	A	768	PO4	P-O2	2.24	1.61	1.54
2	A	765	ATP	C4-N9	-2.19	1.33	1.37
4	B	768	PO4	P-O4	-2.18	1.48	1.54
4	B	767	PO4	P-O4	-2.17	1.48	1.54
4	B	766	PO4	P-O4	-2.15	1.48	1.54
2	B	765	ATP	C4-N9	-2.15	1.33	1.37
4	A	766	PO4	P-O4	-2.12	1.48	1.54
2	B	763	ATP	C4-N9	-2.12	1.33	1.37
2	A	763	ATP	C4-N9	-2.11	1.33	1.37
4	A	768	PO4	P-O4	-2.11	1.48	1.54
4	A	767	PO4	P-O4	-2.11	1.48	1.54
3	B	764	ADP	C4-N9	-2.05	1.33	1.37
3	A	764	ADP	C4-N9	-2.04	1.33	1.37

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	764	ADP	C5-C4-N3	-5.47	119.18	126.72
3	B	764	ADP	C5-C4-N3	-5.33	119.38	126.72
2	B	763	ATP	C5-C4-N3	-5.18	119.58	126.72
2	A	765	ATP	C5-C4-N3	-5.09	119.71	126.72
2	A	763	ATP	C5-C4-N3	-5.04	119.77	126.72
2	B	765	ATP	C5-C4-N3	-4.87	120.01	126.72
2	A	763	ATP	N3-C2-N1	-4.60	121.61	128.58
2	B	765	ATP	N3-C2-N1	-4.56	121.68	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	764	ADP	N3-C2-N1	-4.53	121.73	128.58
2	B	763	ATP	N3-C2-N1	-4.48	121.79	128.58
3	B	764	ADP	N3-C2-N1	-4.46	121.83	128.58
2	A	765	ATP	N3-C2-N1	-4.38	121.95	128.58
2	A	765	ATP	O2A-PA-O5'	-4.05	89.19	107.57
3	A	764	ADP	N3-C4-N9	3.80	133.64	127.17
3	B	764	ADP	N3-C4-N9	3.76	133.56	127.17
2	B	763	ATP	N3-C4-N9	3.68	133.43	127.17
2	A	763	ATP	N3-C4-N9	3.65	133.37	127.17
2	A	765	ATP	O2A-PA-O3A	3.65	117.13	107.27
3	A	764	ADP	C2-N3-C4	3.62	120.67	111.83
2	B	765	ATP	O2A-PA-O5'	-3.61	91.22	107.57
2	A	765	ATP	O2G-PG-O3B	-3.59	92.59	104.64
3	B	764	ADP	C2-N3-C4	3.54	120.47	111.83
2	A	763	ATP	C2-N3-C4	3.49	120.36	111.83
2	B	763	ATP	C2-N3-C4	3.47	120.31	111.83
2	B	765	ATP	O3A-PA-O1A	3.47	121.15	110.70
2	A	765	ATP	N3-C4-N9	3.46	133.05	127.17
2	B	765	ATP	C2-N3-C4	3.43	120.21	111.83
2	B	765	ATP	N3-C4-N9	3.42	132.98	127.17
2	A	765	ATP	C2-N3-C4	3.41	120.16	111.83
2	A	765	ATP	O3G-PG-O3B	-3.38	93.29	104.64
3	A	764	ADP	O2B-PB-O3A	-3.35	93.39	104.64
3	A	764	ADP	O3B-PB-O3A	-3.34	93.43	104.64
2	B	765	ATP	O2A-PA-O3A	3.30	116.20	107.27
2	B	765	ATP	N9-C8-N7	-3.22	109.37	113.94
2	A	765	ATP	C5'-C4'-C3'	-3.22	103.63	115.21
2	B	765	ATP	O5'-PA-O1A	-3.16	96.42	108.94
2	A	765	ATP	O2G-PG-O1G	3.10	122.93	110.83
2	A	763	ATP	N9-C8-N7	-3.03	109.64	113.94
2	A	765	ATP	O3A-PA-O1A	3.01	119.76	110.70
3	A	764	ADP	N9-C8-N7	-2.98	109.71	113.94
2	B	763	ATP	N9-C8-N7	-2.95	109.75	113.94
2	A	765	ATP	O5'-PA-O1A	-2.95	97.25	108.94
3	A	764	ADP	O3B-PB-O1B	2.91	122.16	110.83
3	B	764	ADP	N9-C8-N7	-2.91	109.81	113.94
2	A	765	ATP	N9-C8-N7	-2.90	109.83	113.94
2	B	765	ATP	C5-N7-C8	2.86	107.95	103.45
3	A	764	ADP	C4-C5-N7	-2.84	107.33	110.58
3	A	764	ADP	O2B-PB-O1B	2.82	121.84	110.83
3	A	764	ADP	C5-N7-C8	2.81	107.86	103.45
2	B	765	ATP	C4-C5-N7	-2.79	107.39	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	765	ATP	O3G-PG-O1G	2.71	121.40	110.83
4	A	768	PO4	O4-P-O1	2.71	120.52	110.95
3	B	764	ADP	C5-N7-C8	2.70	107.70	103.45
3	B	764	ADP	C4-C5-N7	-2.70	107.50	110.58
2	A	765	ATP	C4-C5-N7	-2.69	107.51	110.58
4	A	767	PO4	O3-P-O2	-2.65	99.65	107.91
2	A	763	ATP	C5-N7-C8	2.65	107.61	103.45
2	B	763	ATP	C5-N7-C8	2.64	107.60	103.45
2	B	763	ATP	C4-C5-N7	-2.62	107.58	110.58
2	A	765	ATP	C5-N7-C8	2.61	107.55	103.45
4	A	766	PO4	O4-P-O1	2.56	120.00	110.95
2	A	763	ATP	C4-C5-N7	-2.54	107.67	110.58
2	B	765	ATP	C3'-C2'-C1'	-2.53	96.67	101.46
2	B	765	ATP	O4'-C1'-C2'	-2.46	101.35	106.62
2	B	765	ATP	C4-N9-C8	2.41	108.27	105.74
2	A	763	ATP	C4-N9-C8	2.37	108.22	105.74
4	B	767	PO4	O4-P-O1	2.35	119.26	110.95
2	A	763	ATP	C2'-C3'-C4'	-2.30	98.17	102.61
3	A	764	ADP	O3A-PB-O1B	-2.25	99.19	111.04
2	B	763	ATP	C4-N9-C8	2.24	108.09	105.74
2	A	765	ATP	O3B-PG-O1G	-2.23	99.28	111.04
4	A	767	PO4	O4-P-O1	2.21	118.78	110.95
2	B	765	ATP	C4'-O4'-C1'	-2.21	104.59	109.47
4	B	766	PO4	O3-P-O2	-2.18	101.13	107.91
2	A	763	ATP	C2'-C1'-N9	-2.16	107.93	113.30
4	B	766	PO4	O4-P-O1	2.16	118.58	110.95
4	B	768	PO4	O4-P-O1	2.14	118.53	110.95
2	A	765	ATP	O2A-PA-O1A	2.13	122.37	112.44
2	B	765	ATP	O2A-PA-O1A	2.11	122.24	112.44
2	A	765	ATP	O4'-C1'-N9	2.11	112.13	108.09
3	B	764	ADP	C4-N9-C8	2.09	107.93	105.74
3	A	764	ADP	C4-N9-C8	2.08	107.92	105.74
2	B	763	ATP	C2'-C3'-C4'	-2.07	98.60	102.61
3	A	764	ADP	C5'-C4'-C3'	-2.06	107.80	115.21
2	A	765	ATP	C4-N9-C8	2.04	107.88	105.74

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	763	ATP	PB-O3B-PG-O3G
2	A	765	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	A	765	ATP	C5'-O5'-PA-O2A
2	A	765	ATP	C5'-O5'-PA-O3A
2	A	763	ATP	PA-O3A-PB-O1B
3	A	764	ADP	PB-O3A-PA-O1A
2	B	763	ATP	PB-O3A-PA-O1A
2	B	765	ATP	PA-O3A-PB-O1B
2	A	763	ATP	PB-O3A-PA-O2A
3	B	764	ADP	PB-O3A-PA-O1A
2	A	763	ATP	PA-O3A-PB-O2B
3	A	764	ADP	PB-O3A-PA-O2A
2	A	765	ATP	PB-O3A-PA-O2A
2	B	763	ATP	PA-O3A-PB-O2B
2	B	765	ATP	PB-O3A-PA-O1A
3	B	764	ADP	PB-O3A-PA-O2A
2	A	765	ATP	C3'-C4'-C5'-O5'
2	B	763	ATP	PA-O3A-PB-O1B
2	B	763	ATP	PB-O3A-PA-O2A
2	B	765	ATP	PG-O3B-PB-O2B
2	B	765	ATP	PA-O3A-PB-O2B

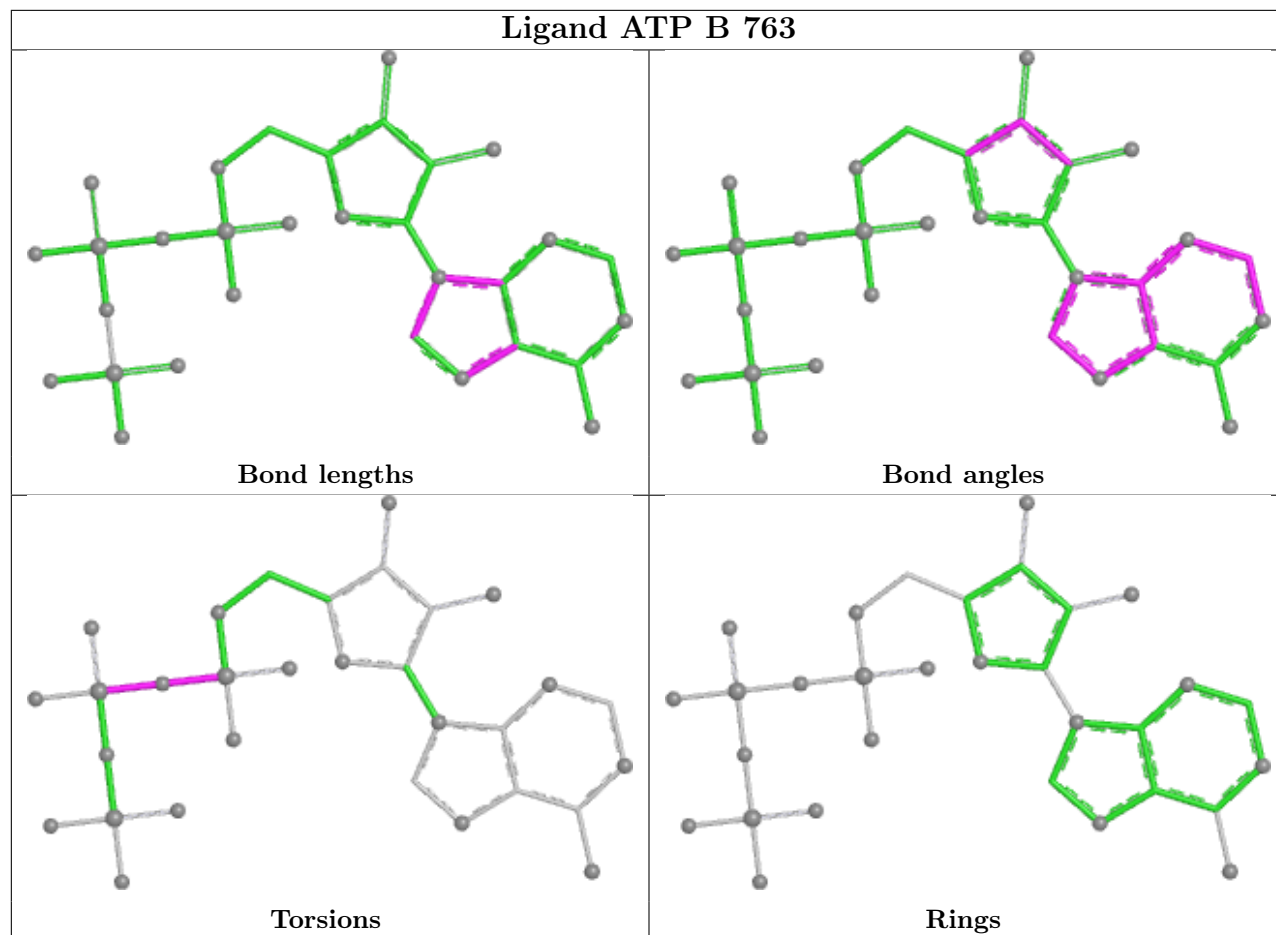
There are no ring outliers.

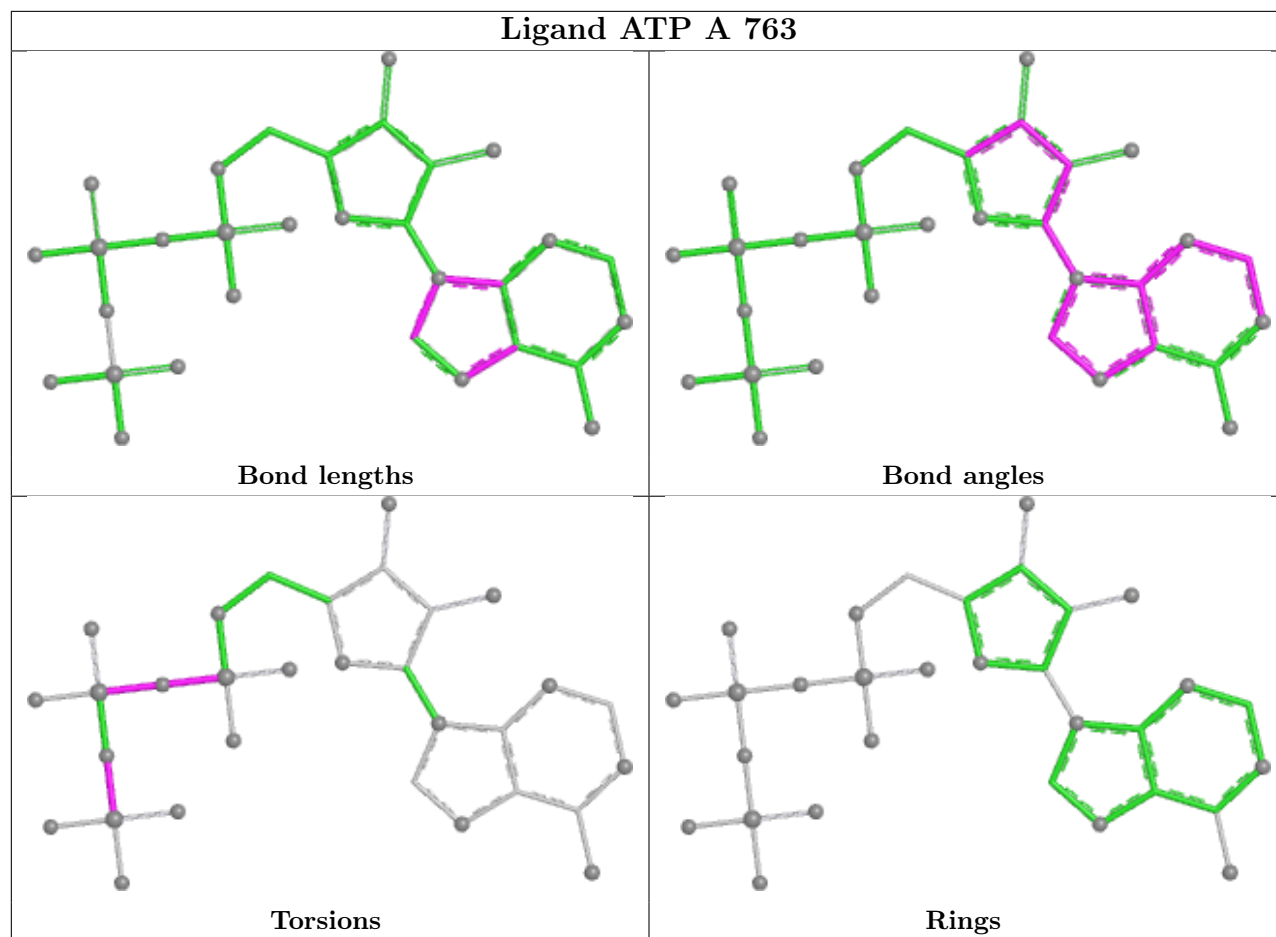
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	763	ATP	1	0
4	A	767	PO4	1	0
2	A	763	ATP	2	0
2	A	765	ATP	3	0
4	B	768	PO4	1	0
3	A	764	ADP	2	0

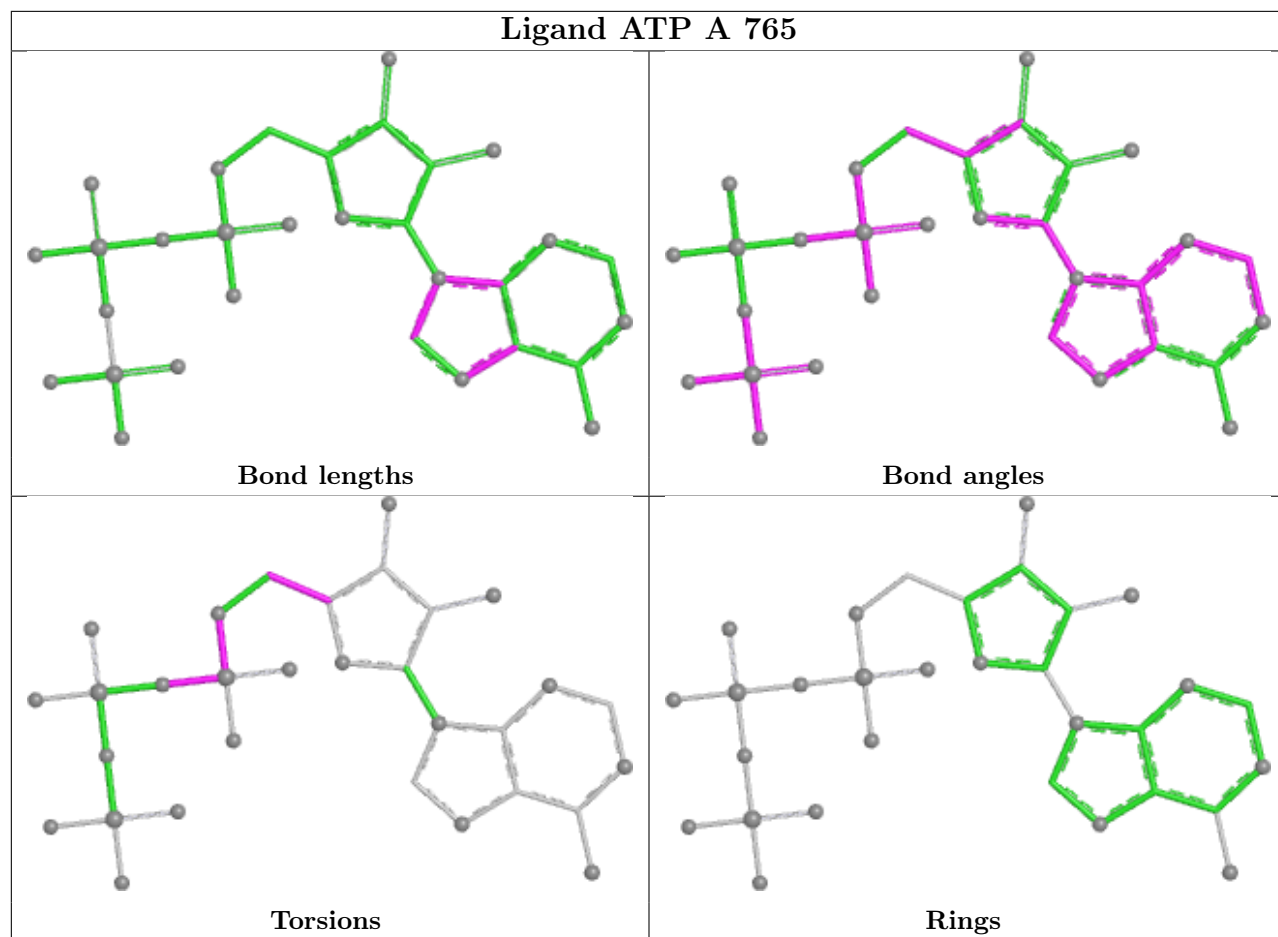
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

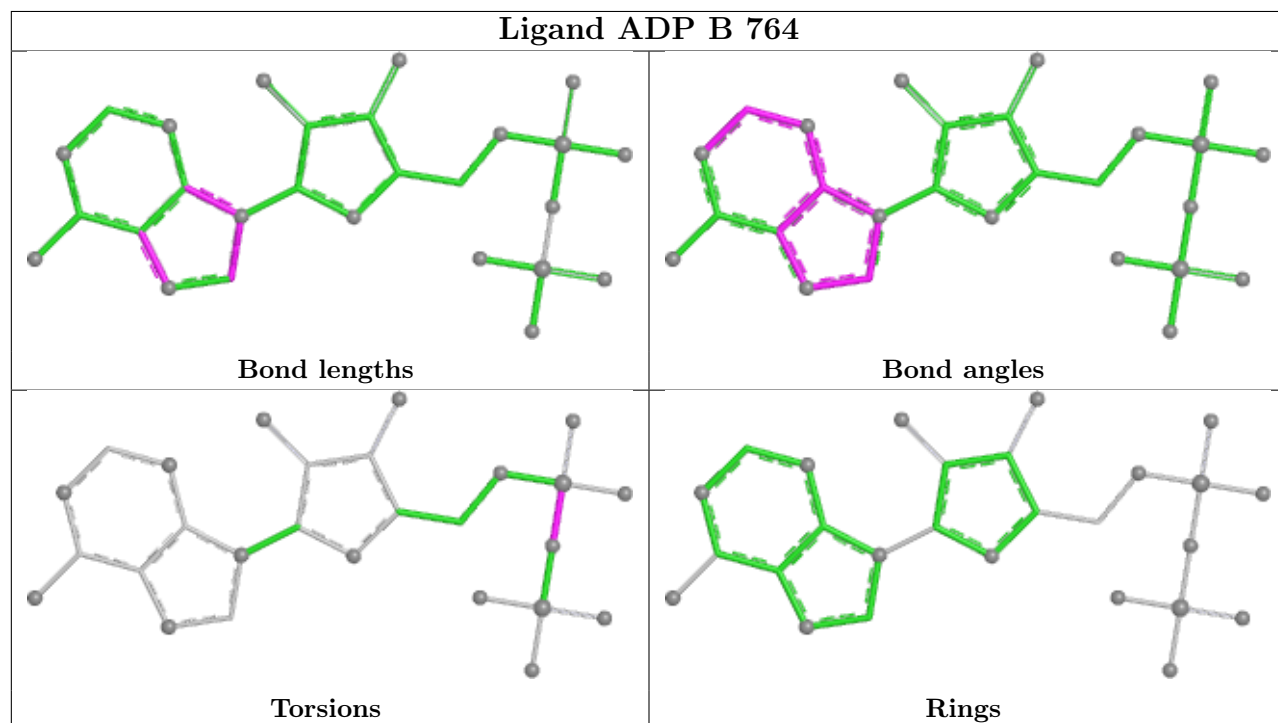


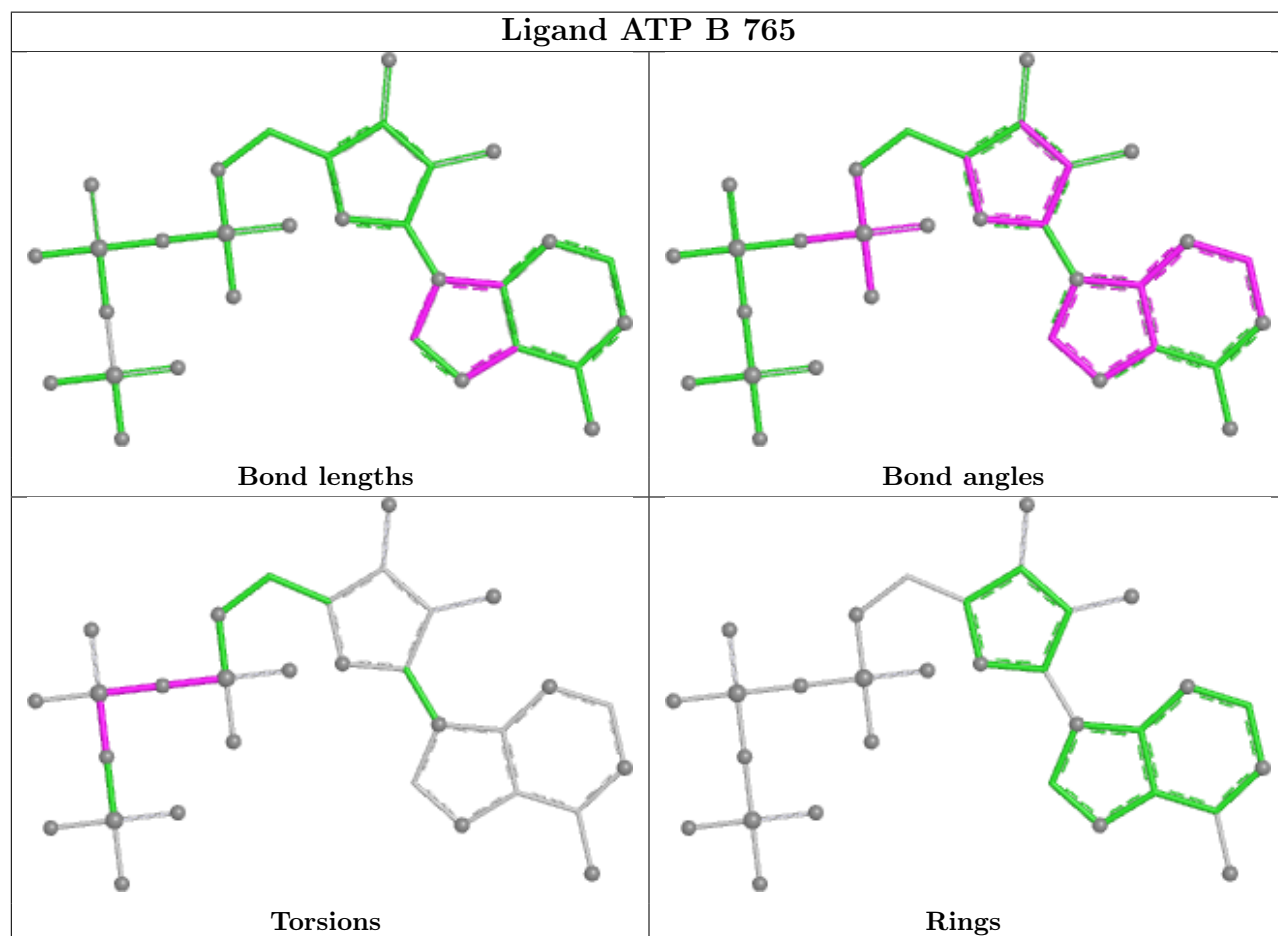
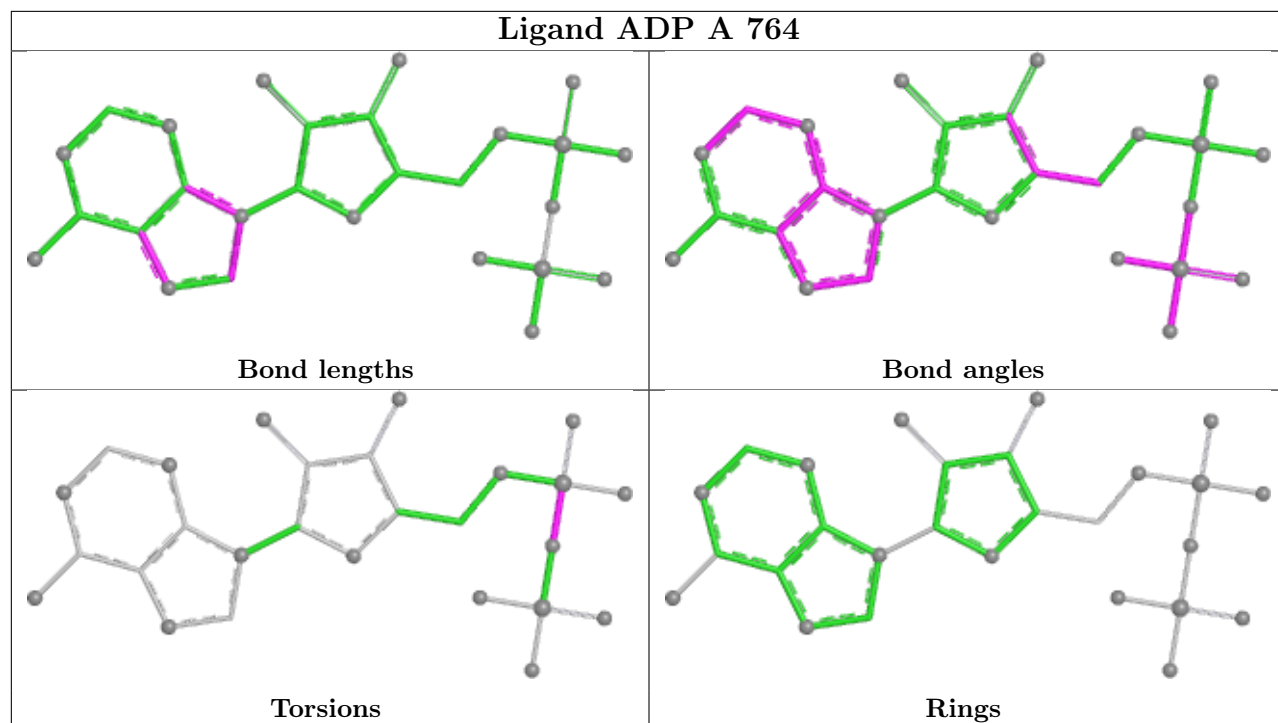


Ligand ATP A 765



Ligand ADP B 764





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	739/762 (96%)	0.08	33 (4%) 38 24	14, 52, 126, 184	76 (10%)
1	B	745/762 (97%)	0.12	35 (4%) 36 23	7, 54, 128, 202	86 (11%)
All	All	1484/1524 (97%)	0.10	68 (4%) 37 23	7, 53, 128, 202	162 (10%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	SER	8.1
1	A	148	GLU	4.8
1	B	563	THR	4.7
1	A	9	ALA	4.5
1	A	155	TYR	4.5
1	A	298	HIS	4.2
1	A	96	GLU	3.9
1	A	662	MET	3.8
1	A	666	GLY	3.7
1	B	665	GLY	3.7
1	B	59	VAL	3.7
1	B	145	ILE	3.6
1	B	147	ALA	3.5
1	B	556	ILE	3.4
1	B	664	GLN	3.4
1	A	89	CYS	3.3
1	A	99	LEU	3.3
1	B	560	ALA	3.2
1	A	90	LYS	3.2
1	B	200	GLN	3.0
1	A	126	ASP	3.0
1	A	195	THR	2.9
1	A	289	TYR	2.8
1	A	559	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	619	THR	2.8
1	A	147	ALA	2.8
1	B	206	GLU	2.7
1	A	245	ARG	2.6
1	B	252	THR	2.6
1	B	154	SER	2.6
1	B	26	ASP	2.5
1	B	392	ARG	2.5
1	B	465	SER	2.5
1	A	123	THR	2.4
1	B	123	THR	2.4
1	B	411	PRO	2.4
1	A	322	MET	2.4
1	B	291	THR	2.4
1	B	697	ASN	2.4
1	A	166	ASP	2.4
1	A	145	ILE	2.4
1	A	380	ASN	2.4
1	B	92	PHE	2.3
1	A	276	SER	2.3
1	A	660	GLY	2.3
1	B	195	THR	2.3
1	B	148	GLU	2.3
1	A	210	ARG	2.3
1	A	137	SER	2.3
1	B	237	ASP	2.3
1	B	171	GLY	2.2
1	B	366	ARG	2.2
1	A	395	ALA	2.2
1	B	87	ALA	2.2
1	B	362	MET	2.2
1	A	128	PHE	2.2
1	B	756	GLU	2.2
1	A	149	GLU	2.1
1	B	196	ALA	2.1
1	A	564	LYS	2.1
1	B	134	ASP	2.1
1	B	135	LEU	2.1
1	A	211	HIS	2.1
1	B	60	ASP	2.1
1	A	619	THR	2.0
1	B	166	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	223	CYS	2.0
1	A	756	GLU	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](#)

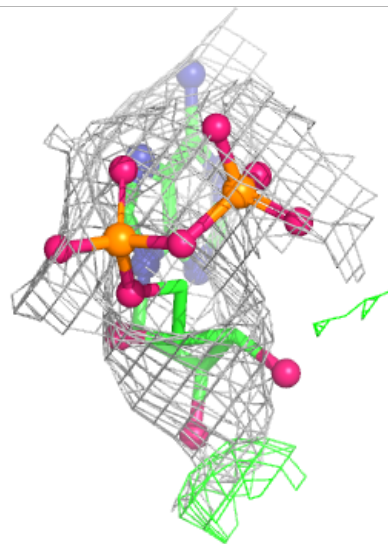
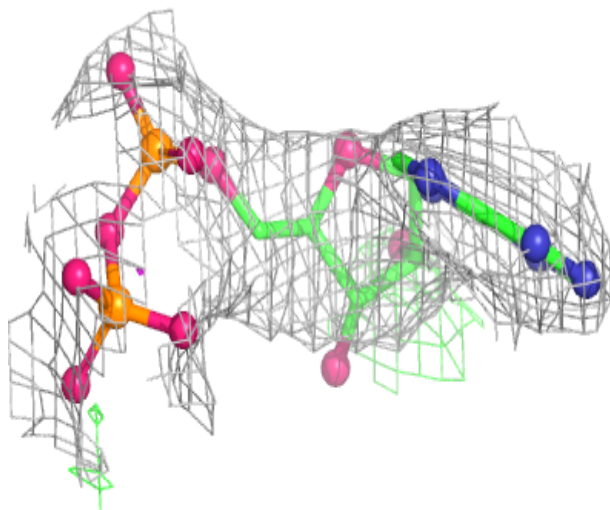
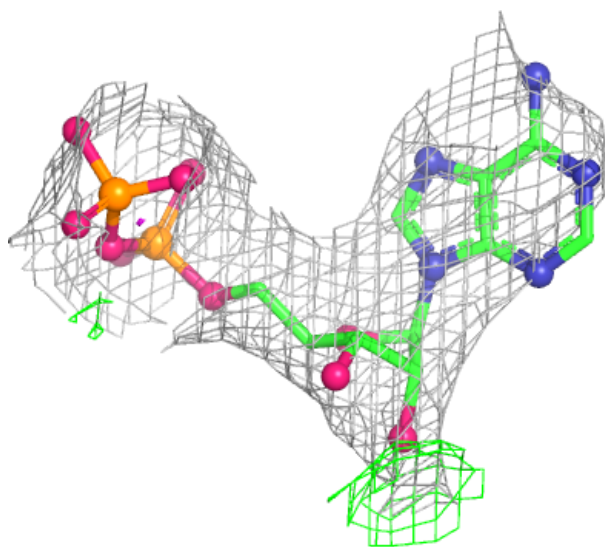
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	A	766	5/5	0.64	0.18	99,99,100,101	0
4	PO4	B	766	5/5	0.74	0.14	91,92,93,94	0
3	ADP	B	764	27/27	0.84	0.18	145,148,154,154	0
3	ADP	A	764	27/27	0.85	0.21	135,138,144,144	0
4	PO4	B	767	5/5	0.90	0.13	66,66,69,71	0
2	ATP	A	763	31/31	0.91	0.09	82,87,97,98	0
2	ATP	B	765	31/31	0.92	0.09	72,77,90,91	0
4	PO4	A	768	5/5	0.92	0.09	55,56,57,58	0
4	PO4	B	768	5/5	0.93	0.09	52,53,55,55	0
2	ATP	B	763	31/31	0.94	0.08	98,100,101,101	0
4	PO4	A	767	5/5	0.94	0.12	60,60,61,63	0
2	ATP	A	765	31/31	0.94	0.07	58,63,77,78	0

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

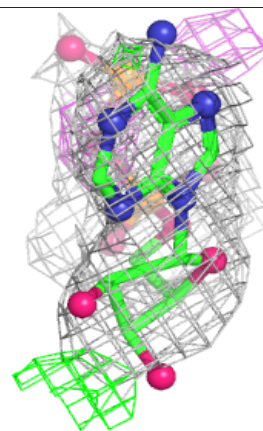
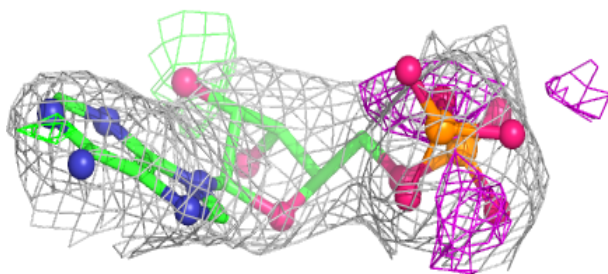
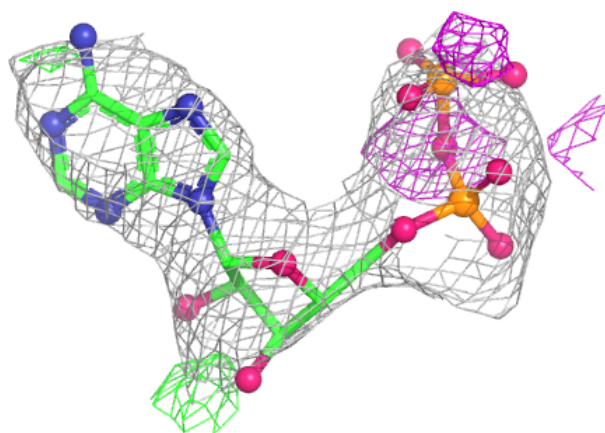
Electron density around ADP B 764:

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



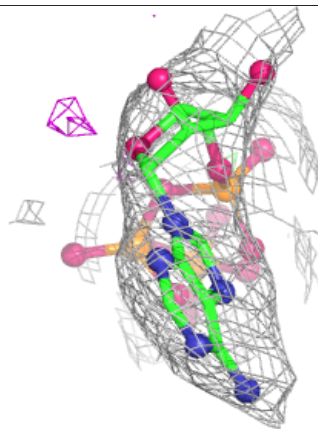
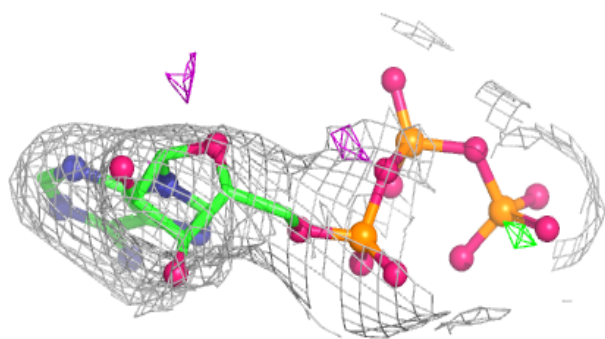
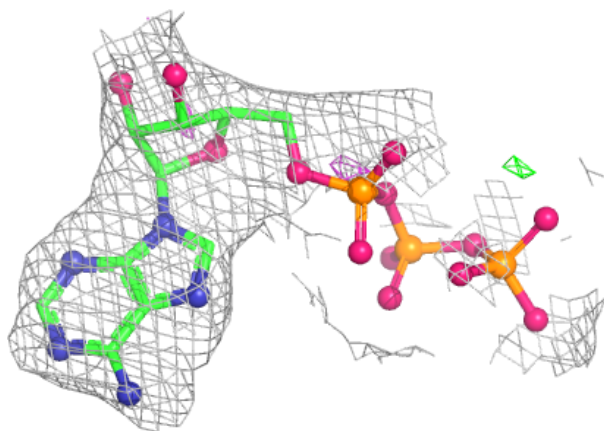
Electron density around ADP A 764:

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



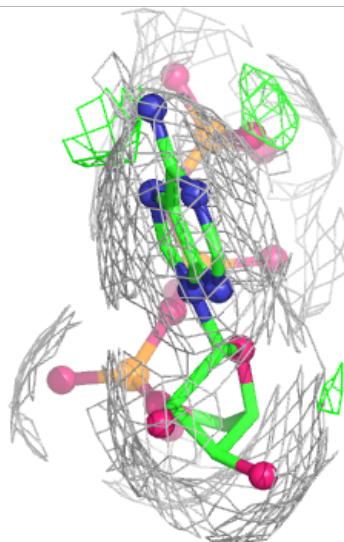
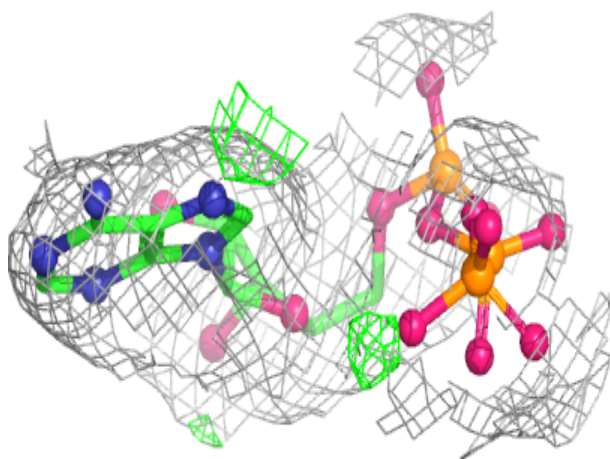
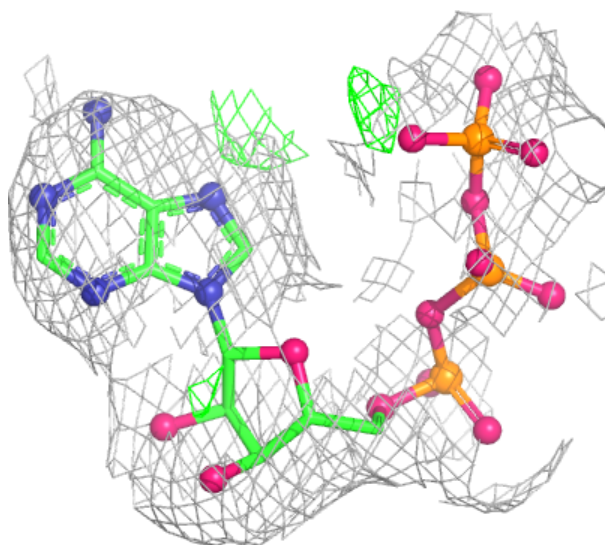
Electron density around ATP A 763:

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



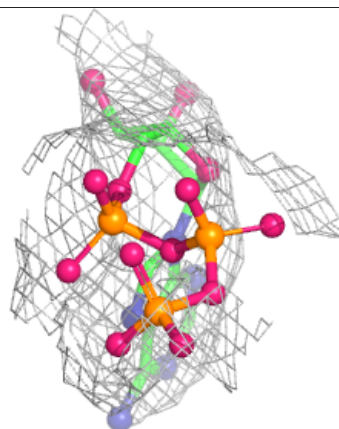
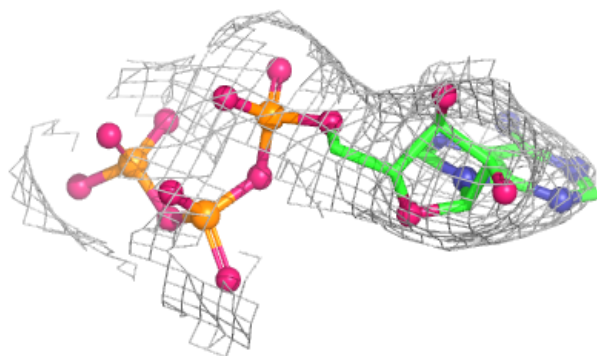
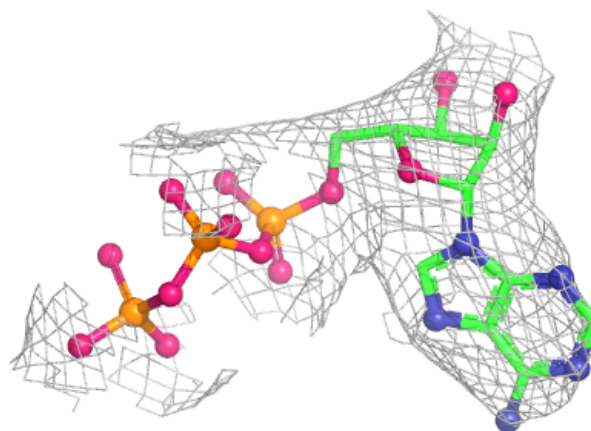
Electron density around ATP B 765:

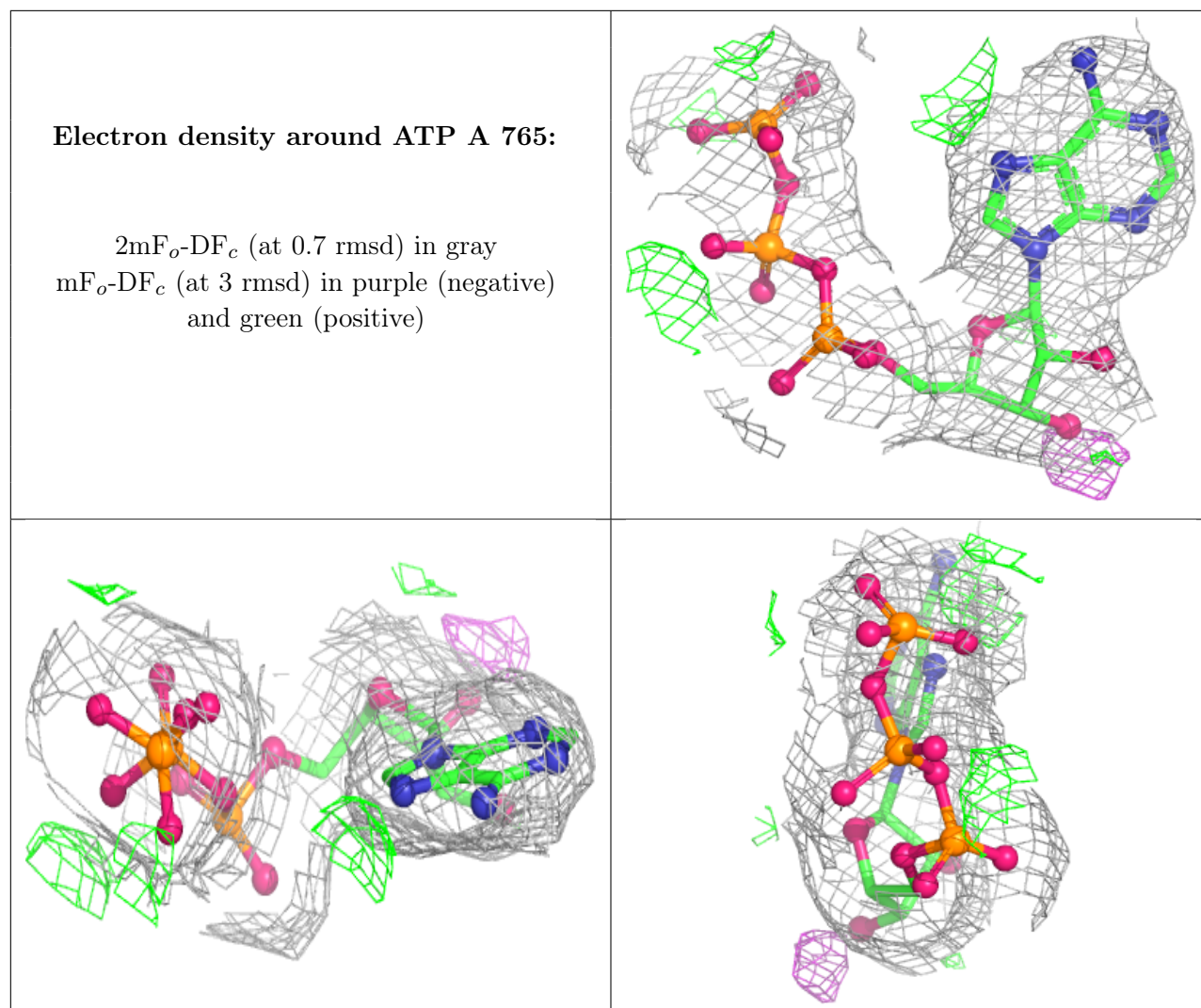
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP B 763:

$2mF_o-DF_c$ (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.