



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:47 AM UTC

PDB ID : 3LC6 / pdb_00003lc6
Title : The alternative conformation structure of isocitrate dehydrogenase kinase/phosphatase from E. Coli
Authors : Zheng, J.; Jia, Z.
Deposited on : 2010-01-09
Resolution : 3.10 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

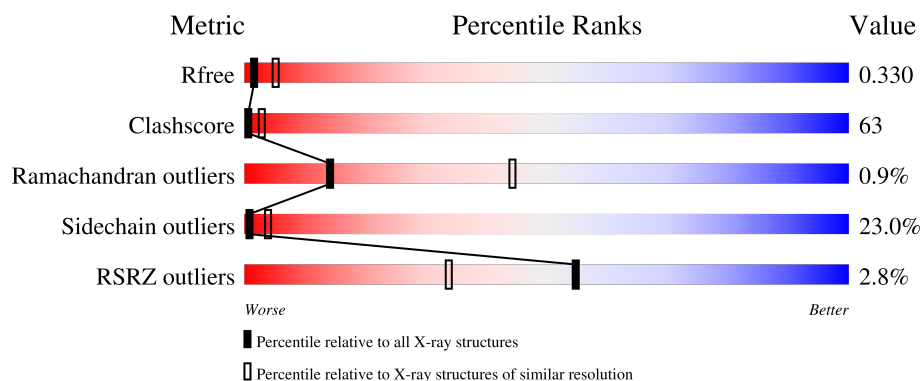
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	578	
1	B	578	

2 Entry composition [i](#)

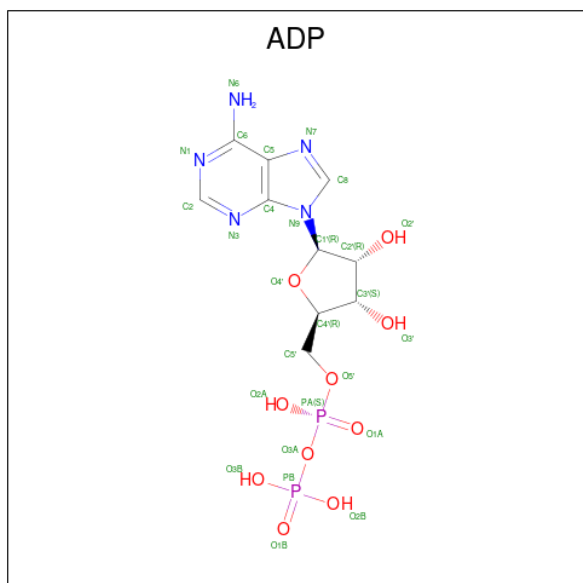
There are 5 unique types of molecules in this entry. The entry contains 9107 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isocitrate dehydrogenase kinase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4526	2906	800	799	21			
1	B	539	Total	C	N	O	S	0	0	0
			4454	2861	785	788	20			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

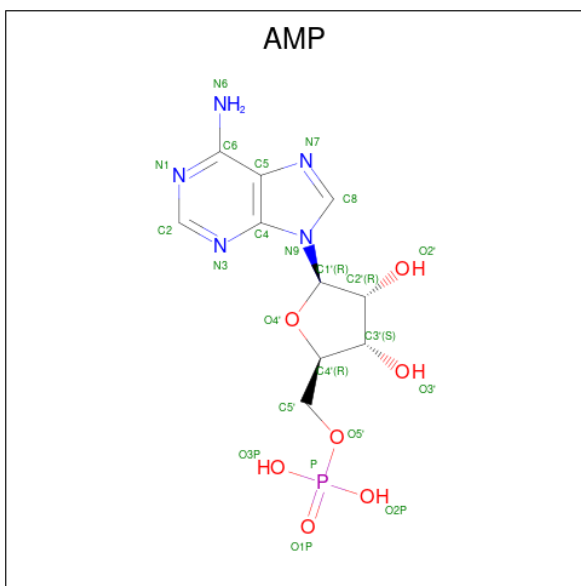


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

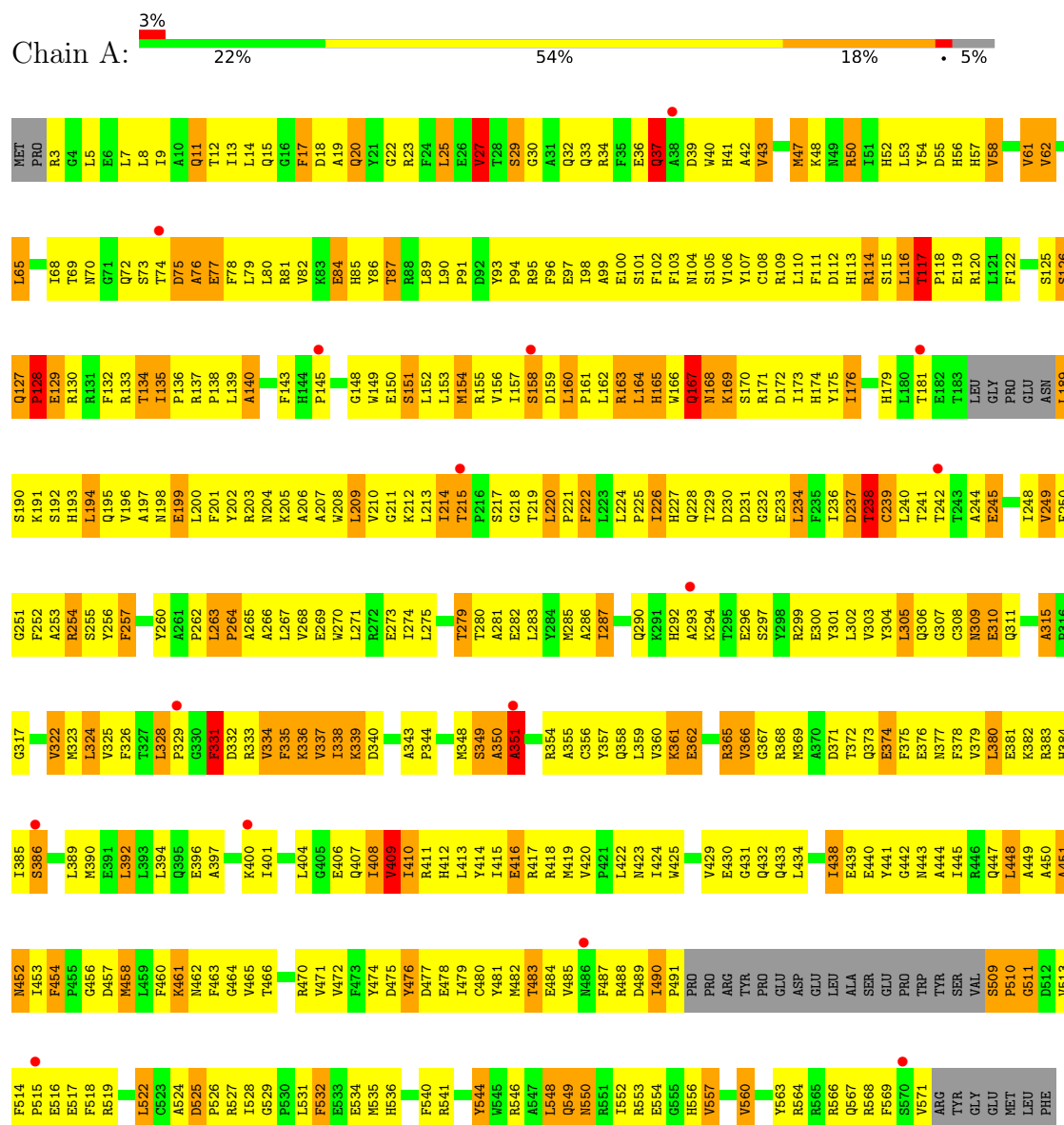
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	45	Total	O	0	0
			45	45		

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: Isocitrate dehydrogenase kinase/phosphatase



- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase



LEU	PHE	F514	F515	E516	F517	F518	F519	R520	H521	L522	D525	I528	G529	F530	L531	F532	M535	H536	A537	D538	L539	F540	R541	A542	D543	Y544	W545	R546	A547	L548	Q549	N550	R551	I552	R553	E554	G555	H556	V557	E558	D559	V560	Y561	A562	A563	Y563	R563	R565	R566	Q567	F568	F569	S570	V571	R572	Y573	G574	GLU	MET				
		A450	A451	N452	L453	F454	P455	G456	D457	N458	L459	F460	K461	N462	F463	G464	V465	T466	R467		R470	V471	V472	F473	Y474	D475	Y476	D477	E478	I479	G480	Y481	N482	T483	E484	V485		D489	L490	PRO	PRO	PRO	PRO	ARG	TYR	PRO	GLU	ASP	GLU	LEU	ALA	R565	R566	Q567	R568	F569	S570	V571	R572	Y573	PRO	G511	
		M390	E391	L392	L393	L394	R395	E396	A397	A398	E399	K400	I401	T402	D403	L404	G405	E406	Q407	I408	V409	I410	R411	H412	L413	Y414	I415	E416	R417	R418	M419	W420	P421	L422	N423	I424	W425	L426	E427	Q428	W429	E430	G431	Q432	Q433	L434	R435	D436	A437	I438	E439	E440	Y441	Q442	R443	A444	T445	R446	Q447	L448	A449		
		P329	G330	F331	D332	R333	V334	F335	K336	V337	I338	K339	D340	K341	F342	ALA	PRO	GLN	LYS	GLU	MET	SER	ALA	A351	H352	V353	R354	A355	C356	R357	Q358	L359	V360	K361	E362	H363	D364	R365	G367	R368	M369	A370	D371	T372	Q373	E374	F375	E376	R377	F378	V379	L380	E381	K382	R383	H384	P387	A388	L389				
		A266	L267	V268	E269	W270	L271	I274	L275	P276	G277	K278	T279	T280	A281	E282	L283	Y284	M285	A286	I287	G288	C289	Q290	K291	H292	A293	K294	T295	E296	S297	Y298	R299	E300	Y301	Y304	L305	Q306	N309	E310	S247	I311	F312	I313	E314	A315	G317	I318	R319	G320	M321	V322	M323	L324	V325	F326	T327	L328					
		Y202	R203	N204	W208	L209	K212	L213	I214	T215	P216	S217	G218	T219	L220	F221	F222	L223	T226	H227	Q228	T229	D230	D231	G232	E233	L234	F235	I236	D237	T238	C239	L240	T241	H242	T243	A244	E245	A246	S247	I248	E249	F250	G251	F252	R254	S255	Y256	F257	M258	Q195	V196	A261	P262	L263	A265							
		ARG	T134	I135	P136	R137	P138	L139	A140	L141	D142	F143	H144	P145	W149	L152	L153	L154	M155	V156	I157	L160	P161	L162	R163	L164	N168	K169	S170	R171	D172	I173	H174	Y175	I176	I177	R178	H179	L180	T181	E182	T183	P186	L189	S192	H193	L194	Q195	V197	N198	E199	L200	P201										
		Q72	S73	T74	D75	F78	L79	L80	R81	V82	H85	H86	T87	R88	L89	P91	D92	Y93	R94	T95	F96	E97	T98	A99	E100	S101	F102	F103	N104	S105	V106	Y107	C108	R109	L110	PHE	D112	H113	R114	S115	L116	T117	P118	E119	R120	L121	F122	I123	F124	S125	S126	Q127	P128	GLU	ARG	PHE							
		MET	P2	R3	G4	L5	E6	L7	L8	R9	A10	Q11	G16	A19	Q20	Y21	F24	L25	E26	V27	T28	S29	Q32	Q33	R34	F35	S101	E36	Q37	A38	D39	W40	V43	Q44	M47	K48	N49	R50	F51	H52	L53	Y54	H57	V58	G59	V61	V62	E63	G64	L65	R66	C67	I68	T69									

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.14Å 133.76Å 187.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10 10.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	83.1 (10.00-3.10) 80.9 (10.00-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	16.46 (at 3.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.287 , 0.332 0.292 , 0.330	Depositor DCC
R_{free} test set	1191 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 81.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	9107	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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: ADP, AMP, MG

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	0.81	8/4643 (0.2%)	1.26	44/6283 (0.7%)
1	B	0.75	4/4567 (0.1%)	1.17	34/6179 (0.6%)
All	All	0.78	12/9210 (0.1%)	1.21	78/12462 (0.6%)

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	1	5
1	B	0	2
All	All	1	7

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	ALA	C-O	7.48	1.32	1.23
1	A	511	GLY	N-CA	6.99	1.55	1.45
1	A	128	PRO	CA-C	-6.46	1.43	1.52
1	B	135	ILE	CA-CB	-5.86	1.50	1.54
1	A	237	ASP	C-O	-5.82	1.17	1.23
1	A	350	ALA	C-N	5.79	1.41	1.33
1	B	278	LYS	CA-C	5.42	1.57	1.53
1	A	351	ALA	N-CA	5.39	1.53	1.46
1	A	140	ALA	CA-CB	-5.36	1.44	1.53
1	B	204	ASN	C-O	-5.29	1.19	1.24
1	A	168	ASN	CA-C	-5.15	1.48	1.53
1	B	239	CYS	CA-C	-5.08	1.46	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	THR	CA-C-N	17.69	137.16	119.82
1	A	117	THR	C-N-CA	17.69	137.16	119.82
1	A	128	PRO	N-CA-C	-16.63	89.69	113.47
1	A	239	CYS	N-CA-C	14.21	130.85	111.24
1	A	191	LYS	N-CA-C	-11.17	98.47	112.88
1	A	130	ARG	N-CA-C	9.97	122.22	111.36
1	A	75	ASP	N-CA-C	-9.78	93.83	108.79
1	B	116	LEU	N-CA-C	9.37	121.57	111.36
1	A	118	PRO	N-CA-C	9.29	125.96	113.98
1	A	349	SER	N-CA-C	9.11	123.64	109.52
1	B	72	GLN	N-CA-C	8.31	120.03	110.97
1	A	487	PHE	N-CA-C	8.24	123.16	108.24
1	B	367	GLY	N-CA-C	-8.15	104.61	115.21
1	A	451	ALA	N-CA-C	-8.12	99.68	110.24
1	A	238	THR	N-CA-C	8.01	129.31	113.29
1	B	321	MET	N-CA-C	-7.99	102.65	111.36
1	B	279	THR	N-CA-C	7.90	123.24	109.80
1	A	454	PHE	CA-C-N	7.84	127.56	119.56
1	A	454	PHE	C-N-CA	7.84	127.56	119.56
1	B	529	GLY	CA-C-N	7.79	129.58	119.84
1	B	529	GLY	C-N-CA	7.79	129.58	119.84
1	A	167	GLN	N-CA-C	7.54	120.60	111.40
1	A	169	LYS	N-CA-C	-7.14	103.58	111.36
1	B	359	LEU	N-CA-C	-7.02	105.25	114.31
1	B	160	LEU	CA-C-N	6.99	127.29	119.32
1	B	160	LEU	C-N-CA	6.99	127.29	119.32
1	A	41	HIS	N-CA-C	-6.89	103.76	111.28
1	B	124	PHE	N-CA-C	6.62	117.88	108.74
1	B	19	ALA	N-CA-C	-6.58	104.15	111.71
1	A	77	GLU	N-CA-C	-6.44	103.17	111.02
1	A	27	VAL	N-CA-C	-6.43	104.06	110.30
1	B	73	SER	N-CA-C	6.37	119.60	110.10
1	B	412	HIS	N-CA-C	6.37	120.33	111.74
1	B	388	ALA	N-CA-C	-6.29	104.34	111.07
1	A	129	GLU	N-CA-C	6.20	117.83	111.14
1	A	509	SER	N-CA-CB	-6.16	100.02	110.50
1	A	409	VAL	N-CA-C	6.12	116.74	108.17
1	B	126	SER	N-CA-C	-6.11	97.78	110.80
1	B	413	LEU	N-CA-C	6.10	118.67	108.73
1	B	252	PHE	N-CA-C	6.06	120.41	112.89
1	A	348	MET	CA-C-N	-6.00	113.16	122.59
1	A	348	MET	C-N-CA	-6.00	113.16	122.59
1	A	315	ALA	CA-C-N	5.95	125.92	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	ALA	C-N-CA	5.95	125.92	120.21
1	B	379	VAL	N-CA-C	5.92	117.12	108.53
1	B	292	HIS	N-CA-C	-5.81	106.17	113.72
1	B	217	SER	N-CA-C	-5.73	106.10	112.57
1	B	135	ILE	CA-C-N	5.72	125.39	119.56
1	B	135	ILE	C-N-CA	5.72	125.39	119.56
1	A	350	ALA	N-CA-C	-5.66	106.04	114.64
1	A	476	TYR	N-CA-C	5.58	119.63	112.26
1	A	15	GLN	N-CA-C	-5.55	106.55	113.38
1	A	47	MET	N-CA-C	-5.53	104.47	111.11
1	A	160	LEU	CA-C-N	5.52	126.73	119.84
1	A	160	LEU	C-N-CA	5.52	126.73	119.84
1	A	348	MET	N-CA-C	-5.50	101.51	110.20
1	A	126	SER	N-CA-C	5.45	117.88	107.75
1	A	331	PHE	N-CA-C	5.42	118.50	110.48
1	A	76	ALA	N-CA-C	-5.40	106.64	113.18
1	B	204	ASN	CB-CA-C	-5.40	109.89	117.23
1	B	181	THR	N-CA-C	5.37	117.22	111.36
1	B	429	VAL	N-CA-C	5.33	114.88	108.06
1	B	564	ARG	N-CA-C	-5.31	102.04	109.96
1	A	251	GLY	N-CA-C	5.28	119.30	112.54
1	A	293	ALA	N-CA-C	-5.27	105.53	111.28
1	B	465	VAL	N-CA-C	5.25	115.87	108.36
1	A	116	LEU	N-CA-C	5.24	116.68	110.19
1	A	490	ILE	N-CA-C	5.19	120.09	108.88
1	A	451	ALA	CA-C-N	-5.18	114.25	122.23
1	A	451	ALA	C-N-CA	-5.18	114.25	122.23
1	B	127	GLN	N-CA-C	-5.16	105.59	112.55
1	B	120	ARG	N-CA-C	5.14	119.51	112.88
1	A	257	PHE	N-CA-C	5.13	118.11	109.95
1	B	168	ASN	N-CA-C	5.12	118.30	111.24
1	B	9	ILE	N-CA-C	5.10	115.32	110.53
1	B	135	ILE	N-CA-C	-5.09	101.55	107.61
1	A	37	GLN	N-CA-C	-5.01	103.72	110.24
1	B	428	GLN	N-CA-C	-5.00	100.15	110.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	239	CYS	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	THR	Peptide
1	A	128	PRO	Peptide
1	A	230	ASP	Peptide
1	A	350	ALA	Peptide
1	A	510	PRO	Peptide
1	B	117	THR	Peptide
1	B	278	LYS	Peptide

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	4526	0	4449	613	7
1	B	4454	0	4376	535	7
2	A	27	0	12	5	0
3	A	1	0	0	0	0
4	B	23	0	12	2	0
5	A	31	0	0	12	0
5	B	45	0	0	11	0
All	All	9107	0	8849	1132	7

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 63.

All (1132) 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:279:THR:OG1	1:A:282:GLU:HG3	1.16	1.29
1:A:128:PRO:HB2	1:A:129:GLU:CA	1.56	1.29
1:A:200:LEU:HD23	1:A:201:PHE:N	1.48	1.29
1:B:550:ASN:O	1:B:554:GLU:HG3	1.31	1.29
1:A:200:LEU:HD23	1:A:200:LEU:C	1.56	1.28
1:A:23:ARG:O	1:A:27:VAL:HG23	1.37	1.25
1:A:128:PRO:CB	1:A:129:GLU:HA	1.57	1.24
1:B:434:LEU:O	1:B:438:ILE:HG23	1.38	1.24
1:B:376:GLU:O	1:B:411:ARG:HA	1.38	1.23
1:A:8:LEU:HD12	5:A:596:HOH:O	1.33	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLU:OE2	2:A:1762:ADP:N6	1.71	1.21
1:B:5:LEU:O	1:B:9:ILE:CG2	1.89	1.20
1:B:228:GLN:HB2	1:B:233:GLU:O	1.37	1.20
1:A:279:THR:OG1	1:A:282:GLU:CG	1.90	1.17
1:A:311:GLN:NE2	5:A:590:HOH:O	1.74	1.17
1:B:237:ASP:O	1:B:238:THR:HG22	1.41	1.16
1:B:124:PHE:HB2	1:B:299:ARG:CG	1.75	1.16
1:B:382:LYS:NZ	1:B:403:ASP:OD1	1.79	1.16
1:A:240:LEU:CD2	1:A:245:GLU:HG3	1.75	1.15
1:B:124:PHE:HB2	1:B:299:ARG:HG2	1.28	1.14
1:B:117:THR:OG1	1:B:118:PRO:HA	1.45	1.12
1:A:308:CYS:C	1:A:309:ASN:HD22	1.56	1.12
1:B:5:LEU:O	1:B:9:ILE:HG22	0.95	1.11
1:A:107:TYR:HE2	1:A:115:SER:HB3	1.16	1.10
1:A:189:LEU:HD23	1:A:189:LEU:C	1.79	1.08
1:B:304:TYR:CD2	1:B:305:LEU:HD12	1.88	1.08
1:B:413:LEU:O	1:B:413:LEU:HD23	1.54	1.07
1:B:203:ARG:NH2	1:B:254:ARG:HD2	1.70	1.07
1:A:168:ASN:HD22	1:A:171:ARG:HB2	1.18	1.07
1:B:124:PHE:CB	1:B:299:ARG:HG2	1.84	1.06
1:A:30:GLY:O	1:A:34:ARG:HG3	1.55	1.06
1:B:253:ALA:CB	1:B:367:GLY:HA2	1.87	1.05
1:B:178:ARG:HA	1:B:181:THR:HG22	1.07	1.04
1:A:155:ARG:O	1:A:159:ASP:OD2	1.74	1.04
1:B:304:TYR:HD2	1:B:305:LEU:CD1	1.69	1.04
1:B:127:GLN:HB3	1:B:128:PRO:HD3	1.38	1.03
1:B:253:ALA:HB3	1:B:367:GLY:HA2	1.35	1.03
1:B:304:TYR:CD2	1:B:305:LEU:CD1	2.42	1.03
1:A:126:SER:O	1:A:128:PRO:HD3	1.57	1.02
1:A:167:GLN:HG2	1:A:233:GLU:HB2	1.39	1.01
1:B:257:PHE:HB2	1:B:286:ALA:O	1.58	1.01
1:A:168:ASN:ND2	1:A:171:ARG:HB2	1.77	0.99
1:A:189:LEU:HD23	1:A:189:LEU:O	1.60	0.99
1:A:240:LEU:HD22	1:A:245:GLU:HG3	1.39	0.99
1:B:404:LEU:HB2	1:B:407:GLN:HE21	1.28	0.99
1:A:238:THR:HG23	1:A:238:THR:O	1.63	0.99
1:A:328:LEU:HD12	1:A:329:PRO:HD2	1.44	0.99
1:A:200:LEU:C	1:A:200:LEU:CD2	2.29	0.98
1:B:538:ASP:OD1	5:B:580:HOH:O	1.82	0.97
1:A:101:SER:HA	1:A:104:ASN:ND2	1.79	0.97
1:B:178:ARG:HA	1:B:181:THR:CG2	1.95	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:CD1	5:A:596:HOH:O	1.99	0.97
1:A:429:VAL:HG12	1:A:433:GLN:OE1	1.64	0.97
1:A:430:GLU:OE2	1:A:527:ARG:NH1	1.97	0.96
1:A:107:TYR:CE2	1:A:115:SER:HB3	2.00	0.96
1:B:61:VAL:O	1:B:65:LEU:N	1.96	0.96
1:A:546:ARG:O	1:A:550:ASN:HB2	1.66	0.95
1:B:516:GLU:O	1:B:519:ARG:HG2	1.64	0.95
1:B:296:GLU:O	1:B:300:GLU:HG3	1.66	0.95
1:B:338:ILE:HG12	1:B:353:VAL:HG21	1.49	0.95
1:A:96:PHE:CE1	1:A:128:PRO:CG	2.51	0.94
1:B:253:ALA:HB1	1:B:367:GLY:C	1.91	0.94
1:B:24:PHE:O	1:B:28:THR:OG1	1.86	0.94
1:B:366:VAL:HG11	1:B:447:GLN:HG2	1.47	0.94
1:B:108:CYS:HB3	1:B:113:HIS:CE1	2.03	0.93
1:B:404:LEU:O	1:B:407:GLN:NE2	2.01	0.93
1:B:327:THR:CG2	1:B:328:LEU:H	1.82	0.92
1:B:541:ARG:NH2	1:B:544:TYR:HB2	1.84	0.92
1:A:305:LEU:HD13	1:A:305:LEU:H	1.30	0.92
1:B:201:PHE:HB3	1:B:257:PHE:CE1	2.04	0.92
1:B:117:THR:OG1	1:B:118:PRO:CA	2.18	0.92
1:B:442:GLY:HA3	1:B:536:HIS:CD2	2.04	0.92
1:B:361:LYS:HE2	1:B:372:THR:O	1.69	0.91
1:A:86:TYR:OH	1:A:99:ALA:O	1.88	0.91
1:A:105:SER:O	1:A:109:ARG:HG2	1.69	0.91
1:A:126:SER:C	1:A:128:PRO:CD	2.43	0.91
1:B:455:PRO:HB2	1:B:458:MET:HB3	1.53	0.91
1:B:267:LEU:O	1:B:271:LEU:HD12	1.70	0.91
1:A:135:ILE:HG12	1:A:266:ALA:HB1	1.52	0.90
1:A:192:SER:HB2	1:A:214:ILE:O	1.71	0.90
1:B:327:THR:HG22	1:B:328:LEU:H	1.35	0.90
1:A:356:CYS:HB2	1:A:476:TYR:O	1.71	0.90
1:A:125:SER:CB	1:A:129:GLU:HG3	2.02	0.90
1:B:382:LYS:HZ3	1:B:403:ASP:CG	1.80	0.90
1:A:189:LEU:HD23	1:A:190:SER:OG	1.71	0.89
1:B:5:LEU:C	1:B:9:ILE:HG22	1.97	0.89
1:B:173:ILE:HG23	5:B:601:HOH:O	1.69	0.89
1:A:454:PHE:HB2	1:A:482:MET:SD	2.13	0.89
1:B:178:ARG:CA	1:B:181:THR:HG22	1.98	0.89
1:A:96:PHE:CE1	1:A:128:PRO:HG2	2.08	0.89
1:B:81:ARG:HG2	1:B:81:ARG:HH21	1.37	0.89
1:B:310:GLU:HG3	1:B:328:LEU:HD23	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ALA:HB1	1:B:558:GLU:CG	2.03	0.88
1:A:193:HIS:NE2	1:A:214:ILE:HG21	1.88	0.88
1:B:228:GLN:CB	1:B:233:GLU:O	2.21	0.88
1:B:304:TYR:HD2	1:B:305:LEU:HD12	1.28	0.88
1:B:551:ARG:O	1:B:556:HIS:HB3	1.72	0.88
1:A:309:ASN:HD22	1:A:309:ASN:N	1.68	0.88
1:B:535:MET:O	5:B:580:HOH:O	1.92	0.88
1:A:65:LEU:O	1:A:69:THR:OG1	1.90	0.88
1:A:356:CYS:CB	1:A:476:TYR:O	2.22	0.88
1:B:137:ARG:HB3	1:B:138:PRO:HD2	1.54	0.87
1:A:132:PHE:O	1:A:134:THR:HG23	1.74	0.87
1:A:193:HIS:CD2	1:A:214:ILE:HG21	2.09	0.87
1:B:336:LYS:HD2	1:B:416:GLU:OE2	1.74	0.87
1:B:327:THR:HG22	1:B:328:LEU:N	1.87	0.87
1:A:23:ARG:O	1:A:27:VAL:CG2	2.23	0.86
1:A:75:ASP:HB2	1:A:77:GLU:HG2	1.53	0.86
1:A:443:ASN:O	1:A:447:GLN:HG3	1.76	0.86
1:A:381:GLU:O	1:A:385:ILE:HG12	1.74	0.86
1:B:284:TYR:CE1	1:B:292:HIS:HD2	1.93	0.86
1:A:489:ASP:HA	1:A:514:PHE:CD1	2.11	0.86
1:A:252:PHE:CE2	1:A:417:ARG:HD2	2.11	0.85
1:A:221:PRO:O	1:A:241:THR:HG23	1.77	0.85
1:A:96:PHE:CE1	1:A:128:PRO:HG3	2.11	0.85
1:A:294:LYS:HG3	1:A:373:GLN:HG2	1.59	0.85
1:A:126:SER:C	1:A:128:PRO:HD2	2.02	0.84
1:B:127:GLN:HB3	1:B:128:PRO:CD	2.07	0.84
1:A:167:GLN:OE1	1:A:167:GLN:HA	1.77	0.84
1:B:482:MET:HE2	1:B:545:TRP:HZ3	1.42	0.84
1:A:240:LEU:HD22	1:A:245:GLU:CG	2.07	0.83
1:B:90:LEU:HD22	1:B:96:PHE:HB2	1.58	0.83
1:A:444:ALA:O	1:A:448:LEU:HD22	1.78	0.83
1:B:253:ALA:CB	1:B:367:GLY:CA	2.56	0.83
1:A:113:HIS:HB2	1:A:376:GLU:HB3	1.61	0.82
1:A:279:THR:OG1	1:A:282:GLU:CD	2.21	0.82
1:A:465:VAL:HA	1:A:470:ARG:O	1.79	0.82
1:A:192:SER:CB	1:A:214:ILE:O	2.27	0.82
1:A:525:ASP:HB3	1:A:528:ILE:HG12	1.61	0.82
1:B:7:LEU:O	1:B:11:GLN:HG2	1.79	0.82
1:A:335:PHE:HB3	1:A:413:LEU:HD11	1.60	0.82
5:A:596:HOH:O	1:B:60:LEU:HD11	1.78	0.82
1:A:125:SER:HB3	1:A:129:GLU:HG3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ASP:OD1	1:A:516:GLU:HB3	1.80	0.82
1:B:124:PHE:CB	1:B:299:ARG:CG	2.52	0.82
1:A:257:PHE:N	1:A:286:ALA:O	2.10	0.81
1:B:108:CYS:HB3	1:B:113:HIS:ND1	1.95	0.81
1:A:449:ALA:HB1	1:A:482:MET:HE2	1.62	0.81
1:B:95:ARG:HH22	1:B:262:PRO:HB3	1.43	0.81
1:B:482:MET:O	1:B:549:GLN:NE2	2.13	0.81
1:A:139:LEU:C	1:A:198:ASN:OD1	2.24	0.81
1:A:332:ASP:OD1	1:A:333:ARG:HG3	1.80	0.81
1:B:89:LEU:C	1:B:91:PRO:HD3	2.05	0.81
1:B:427:GLU:C	1:B:429:VAL:H	1.83	0.81
1:A:338:ILE:N	1:A:338:ILE:HD12	1.96	0.81
1:A:338:ILE:O	1:A:400:LYS:HD2	1.80	0.81
1:A:107:TYR:HE2	1:A:115:SER:CB	1.94	0.81
1:A:20:GLN:HA	1:A:57:HIS:CD2	2.16	0.81
1:A:325:VAL:HG11	2:A:1762:ADP:O4'	1.80	0.80
1:A:294:LYS:HG3	1:A:373:GLN:CG	2.10	0.80
1:B:538:ASP:HB3	1:B:541:ARG:NH2	1.95	0.80
1:A:203:ARG:O	5:A:594:HOH:O	1.99	0.80
1:A:382:LYS:HB3	1:A:406:GLU:O	1.82	0.80
1:B:450:ALA:HB1	1:B:558:GLU:HG2	1.64	0.80
1:A:96:PHE:HE1	1:A:128:PRO:HG2	1.43	0.80
1:A:366:VAL:HG13	1:A:560:VAL:HB	1.64	0.80
1:A:189:LEU:C	1:A:189:LEU:CD2	2.54	0.80
1:A:252:PHE:CD2	1:A:417:ARG:HD2	2.17	0.80
1:B:153:LEU:O	1:B:157:ILE:HD12	1.82	0.80
1:A:47:MET:SD	1:A:362:GLU:O	2.40	0.80
1:A:238:THR:O	1:A:238:THR:CG2	2.29	0.80
1:B:245:GLU:O	1:B:248:ILE:HG22	1.82	0.79
1:A:167:GLN:CG	1:A:233:GLU:HB2	2.13	0.79
1:B:438:ILE:HG13	1:B:439:GLU:N	1.97	0.79
1:A:189:LEU:O	1:A:189:LEU:CD2	2.30	0.79
1:B:201:PHE:HB3	1:B:257:PHE:CD1	2.17	0.79
1:B:366:VAL:CG1	1:B:447:GLN:HG2	2.11	0.79
1:A:126:SER:O	1:A:128:PRO:CD	2.30	0.79
1:A:400:LYS:NZ	1:A:412:HIS:NE2	2.31	0.79
1:A:268:VAL:HG13	1:A:283:LEU:HB3	1.63	0.79
1:B:100:GLU:O	1:B:104:ASN:ND2	2.16	0.79
1:B:32:GLN:OE1	5:B:615:HOH:O	2.01	0.78
1:B:208:TRP:CE3	1:B:223:LEU:HD22	2.18	0.78
1:B:97:GLU:O	1:B:100:GLU:HG2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:GLY:HA2	1:B:424:ILE:HD11	1.64	0.78
1:A:108:CYS:O	1:A:113:HIS:N	2.15	0.78
1:A:189:LEU:CD2	1:A:190:SER:OG	2.30	0.78
1:A:509:SER:N	1:A:510:PRO:CD	2.47	0.78
1:A:47:MET:HG3	1:A:48:LYS:H	1.48	0.78
1:A:167:GLN:OE1	1:A:167:GLN:CA	2.30	0.78
1:A:305:LEU:H	1:A:305:LEU:CD1	1.96	0.77
1:B:322:VAL:HG11	1:B:475:ASP:OD2	1.85	0.77
1:A:340:ASP:OD1	1:A:400:LYS:HG3	1.84	0.77
1:B:208:TRP:CE3	1:B:223:LEU:CD2	2.68	0.77
1:B:237:ASP:O	1:B:238:THR:CG2	2.29	0.77
1:B:304:TYR:HD2	1:B:305:LEU:HD13	1.48	0.77
1:B:387:PRO:HA	1:B:390:MET:CB	2.14	0.77
1:B:366:VAL:HG11	1:B:447:GLN:CG	2.14	0.77
1:A:128:PRO:HB2	1:A:129:GLU:HA	0.80	0.77
1:B:29:SER:HB3	1:B:260:TYR:CD1	2.20	0.77
1:B:61:VAL:HG23	1:B:62:VAL:N	2.00	0.77
1:B:304:TYR:CD2	1:B:305:LEU:HD13	2.20	0.77
1:A:488:ARG:O	1:A:514:PHE:CE1	2.37	0.77
1:B:413:LEU:HD23	1:B:413:LEU:C	2.10	0.77
1:B:550:ASN:O	1:B:554:GLU:CG	2.24	0.77
1:A:254:ARG:C	1:A:365:ARG:NH2	2.43	0.76
1:A:125:SER:HB2	1:A:129:GLU:HG3	1.67	0.76
1:B:368:ARG:NH1	5:B:590:HOH:O	2.17	0.76
1:A:47:MET:HG3	1:A:48:LYS:N	2.00	0.76
1:A:381:GLU:HB2	1:A:384:HIS:HB2	1.67	0.76
1:B:203:ARG:HH21	1:B:254:ARG:HD2	1.49	0.76
1:B:418:ARG:O	1:B:418:ARG:HG3	1.84	0.76
1:A:137:ARG:NH2	1:B:199:GLU:OE1	2.19	0.75
1:B:68:ILE:HG13	1:B:69:THR:H	1.51	0.75
1:A:166:TRP:C	1:A:167:GLN:OE1	2.30	0.75
1:A:423:ASN:OD1	1:A:461:LYS:CB	2.35	0.75
1:B:296:GLU:O	1:B:300:GLU:CG	2.35	0.75
1:B:90:LEU:N	1:B:91:PRO:HD3	2.02	0.75
1:A:268:VAL:HG13	1:A:283:LEU:CB	2.17	0.74
1:A:304:TYR:CE2	1:A:328:LEU:HD21	2.21	0.74
1:B:95:ARG:NH2	1:B:262:PRO:HB3	2.02	0.74
1:B:564:ARG:HH21	1:B:564:ARG:HG3	1.52	0.74
1:B:253:ALA:HB3	1:B:367:GLY:CA	2.13	0.74
1:B:48:LYS:HE2	1:B:362:GLU:CD	2.12	0.74
1:B:326:PHE:HE2	1:B:337:VAL:HG12	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:HIS:CD2	1:A:296:GLU:HG2	2.23	0.74
1:B:81:ARG:HH21	1:B:81:ARG:CG	2.00	0.74
1:B:450:ALA:CB	1:B:558:GLU:HG2	2.17	0.74
1:A:76:ALA:HA	1:A:79:LEU:HB2	1.68	0.74
1:B:275:LEU:O	1:B:277:GLY:N	2.21	0.74
1:B:376:GLU:HA	1:B:412:HIS:H	1.52	0.73
1:A:108:CYS:HB3	1:A:113:HIS:CD2	2.23	0.73
1:B:25:LEU:HB3	1:B:260:TYR:CE1	2.23	0.73
1:A:128:PRO:CG	1:A:129:GLU:HA	2.18	0.73
1:A:304:TYR:HE2	1:A:328:LEU:HD21	1.53	0.73
1:A:420:VAL:HG23	1:A:420:VAL:O	1.86	0.73
1:A:361:LYS:NZ	1:A:372:THR:OG1	2.22	0.73
1:A:90:LEU:N	1:A:91:PRO:HD3	2.03	0.73
1:A:101:SER:HA	1:A:104:ASN:HD22	1.52	0.73
1:B:387:PRO:HA	1:B:390:MET:HB2	1.69	0.73
1:B:525:ASP:HB3	1:B:528:ILE:HD12	1.70	0.73
1:B:541:ARG:HH22	1:B:544:TYR:HB2	1.51	0.73
1:A:338:ILE:HD12	1:A:338:ILE:H	1.54	0.73
1:A:107:TYR:CE2	1:A:115:SER:CB	2.71	0.72
1:A:192:SER:HB3	1:A:215:THR:HA	1.71	0.72
1:A:452:ASN:OD1	1:A:552:ILE:HG21	1.89	0.72
1:A:452:ASN:O	1:A:453:ILE:HD13	1.89	0.72
1:B:253:ALA:CB	1:B:367:GLY:C	2.62	0.72
1:A:429:VAL:CG1	1:A:433:GLN:OE1	2.37	0.72
1:A:440:GLU:HB3	1:A:471:VAL:HG23	1.71	0.72
1:B:397:ALA:O	1:B:401:ILE:HD12	1.89	0.72
1:B:399:GLU:OE2	5:B:617:HOH:O	2.06	0.72
1:B:242:THR:O	1:B:245:GLU:HG3	1.88	0.72
1:A:371:ASP:CG	1:A:372:THR:H	1.98	0.72
1:B:118:PRO:HD2	1:B:119:GLU:H	1.55	0.72
1:A:549:GLN:O	1:A:553:ARG:HG3	1.90	0.72
1:B:323:MET:SD	1:B:338:ILE:HG13	2.29	0.72
1:B:372:THR:HA	1:B:415:ILE:O	1.90	0.72
1:A:454:PHE:CZ	1:A:513:VAL:HG11	2.25	0.71
1:B:275:LEU:O	1:B:275:LEU:HG	1.88	0.71
1:B:438:ILE:CG1	1:B:439:GLU:N	2.53	0.71
1:B:253:ALA:HB1	1:B:367:GLY:CA	2.20	0.71
1:A:488:ARG:O	1:A:514:PHE:CD1	2.43	0.71
1:A:488:ARG:HH21	1:A:490:ILE:HB	1.54	0.71
1:B:215:THR:O	1:B:218:GLY:O	2.09	0.71
1:A:524:ALA:O	1:A:526:PRO:HD3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:HIS:O	1:A:234:LEU:HB2	1.91	0.71
1:A:328:LEU:HD12	1:A:329:PRO:CD	2.18	0.71
1:B:229:THR:N	1:B:233:GLU:OE2	2.23	0.71
1:A:419:MET:HE1	1:A:472:VAL:HB	1.71	0.71
1:A:458:MET:HE3	5:A:601:HOH:O	1.90	0.70
1:A:462:ASN:CG	1:A:475:ASP:OD2	2.34	0.70
1:B:122:PHE:N	1:B:122:PHE:CD2	2.58	0.70
1:B:352:HIS:O	1:B:356:CYS:HB2	1.91	0.70
1:A:308:CYS:C	1:A:309:ASN:ND2	2.41	0.70
1:A:430:GLU:HA	1:A:434:LEU:HB2	1.72	0.70
1:A:461:LYS:H	1:A:461:LYS:HD3	1.56	0.70
1:A:30:GLY:O	1:A:34:ARG:CG	2.38	0.70
1:B:229:THR:HG22	1:B:233:GLU:OE2	1.90	0.70
1:A:97:GLU:OE2	1:A:265:ALA:HB2	1.92	0.70
1:A:48:LYS:HG2	1:A:362:GLU:HB2	1.72	0.70
1:B:354:ARG:NE	1:B:374:GLU:OE2	2.25	0.70
1:A:322:VAL:O	1:A:339:LYS:HG3	1.91	0.70
1:A:463:PHE:HB3	1:A:471:VAL:HG12	1.72	0.70
1:B:208:TRP:HE3	1:B:223:LEU:CD2	2.03	0.70
1:B:122:PHE:H	1:B:122:PHE:HD2	1.38	0.69
1:A:228:GLN:HA	1:A:234:LEU:HA	1.74	0.69
1:A:128:PRO:HB2	1:A:129:GLU:C	2.16	0.69
1:A:281:ALA:O	1:A:285:MET:HG3	1.92	0.69
1:B:438:ILE:HD13	1:B:531:LEU:HB3	1.72	0.69
1:A:132:PHE:C	1:A:134:THR:HG23	2.18	0.69
1:A:357:TYR:CE1	1:A:476:TYR:HD2	2.09	0.69
1:A:376:GLU:O	1:A:411:ARG:HA	1.90	0.69
1:A:77:GLU:HG3	1:A:78:PHE:N	2.06	0.69
1:A:95:ARG:NH2	1:B:26:GLU:HG2	2.06	0.69
1:A:279:THR:HG1	1:A:282:GLU:CD	2.00	0.69
1:A:449:ALA:CB	1:A:482:MET:HE2	2.21	0.69
1:B:117:THR:HG1	1:B:118:PRO:HA	1.54	0.69
1:B:220:LEU:HD12	1:B:221:PRO:HD2	1.74	0.69
1:B:48:LYS:O	1:B:52:HIS:ND1	2.25	0.69
1:B:412:HIS:CG	1:B:412:HIS:O	2.46	0.69
1:B:87:THR:CG2	1:B:122:PHE:HE1	2.05	0.69
1:B:270:TRP:CE3	1:B:271:LEU:HG	2.28	0.69
1:B:274:ILE:HG13	1:B:275:LEU:H	1.56	0.69
1:B:427:GLU:C	1:B:429:VAL:N	2.51	0.69
1:A:93:TYR:O	1:A:96:PHE:HB3	1.91	0.69
1:B:68:ILE:HG13	1:B:69:THR:N	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:O	1:B:163:ARG:NH1	2.25	0.69
1:A:153:LEU:CD2	1:A:176:ILE:HG21	2.23	0.69
1:A:139:LEU:O	1:A:198:ASN:OD1	2.10	0.68
1:A:200:LEU:HD23	1:A:201:PHE:CA	2.22	0.68
1:A:255:SER:HA	1:A:365:ARG:HH21	1.58	0.68
1:A:292:HIS:HD2	1:A:292:HIS:O	1.76	0.68
1:B:544:TYR:O	1:B:548:LEU:HB3	1.94	0.68
1:A:94:PRO:HB2	1:A:263:LEU:HD21	1.76	0.68
1:A:454:PHE:HZ	1:A:513:VAL:HG11	1.59	0.68
1:B:324:LEU:O	1:B:337:VAL:HG13	1.94	0.68
1:B:334:VAL:O	1:B:415:ILE:HG23	1.94	0.68
1:B:21:TYR:O	1:B:24:PHE:HB3	1.94	0.68
1:B:152:LEU:N	1:B:152:LEU:HD22	2.08	0.68
1:A:58:VAL:O	1:A:62:VAL:HB	1.93	0.67
1:B:124:PHE:CB	1:B:299:ARG:HD3	2.25	0.67
1:B:137:ARG:HB3	1:B:138:PRO:CD	2.23	0.67
1:B:419:MET:HE1	1:B:472:VAL:CG2	2.24	0.67
1:B:54:TYR:OH	1:B:102:PHE:HA	1.93	0.67
1:B:93:TYR:HB3	1:B:96:PHE:HB3	1.75	0.67
1:B:118:PRO:CD	1:B:119:GLU:H	2.08	0.67
1:A:95:ARG:NH2	1:B:26:GLU:OE1	2.27	0.67
1:B:107:TYR:OH	1:B:115:SER:O	2.10	0.67
1:B:203:ARG:NH2	1:B:254:ARG:CD	2.53	0.67
1:A:343:ALA:HB3	1:A:344:PRO:HD3	1.76	0.67
1:A:52:HIS:NE2	1:A:362:GLU:OE1	2.26	0.67
1:B:97:GLU:OE1	1:B:265:ALA:HB2	1.95	0.67
1:B:376:GLU:O	1:B:411:ARG:CA	2.31	0.67
1:A:255:SER:HA	1:A:365:ARG:NH2	2.11	0.66
1:A:411:ARG:O	1:A:412:HIS:CD2	2.48	0.66
1:B:323:MET:HG3	1:B:338:ILE:HA	1.77	0.66
1:A:434:LEU:HD11	1:A:528:ILE:HG22	1.78	0.66
1:A:55:ASP:HA	1:A:58:VAL:CG1	2.25	0.66
1:B:65:LEU:O	1:B:68:ILE:HG12	1.96	0.66
1:B:274:ILE:HG13	1:B:275:LEU:N	2.09	0.66
1:A:222:PHE:HD2	1:A:222:PHE:O	1.79	0.66
1:B:448:LEU:HD13	1:B:453:ILE:CG2	2.26	0.66
1:A:97:GLU:HB2	1:A:292:HIS:HE1	1.60	0.66
1:B:215:THR:C	1:B:217:SER:H	2.04	0.66
1:A:132:PHE:C	1:A:134:THR:H	2.02	0.66
1:A:254:ARG:O	1:A:365:ARG:NH2	2.29	0.66
1:A:279:THR:CB	1:A:282:GLU:HG3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:TYR:C	1:A:415:ILE:HD12	2.19	0.66
1:A:451:ALA:O	1:A:453:ILE:N	2.29	0.66
1:B:419:MET:HE1	1:B:472:VAL:HG22	1.76	0.65
1:A:139:LEU:HD21	1:A:267:LEU:HD13	1.78	0.65
1:A:404:LEU:N	1:A:407:GLN:O	2.28	0.65
1:A:167:GLN:OE1	1:A:167:GLN:N	2.29	0.65
1:A:220:LEU:HG	1:A:221:PRO:HD3	1.78	0.65
1:B:123:ILE:O	1:B:123:ILE:HG12	1.95	0.65
1:B:366:VAL:HG12	1:B:366:VAL:O	1.96	0.65
1:A:337:VAL:HG22	1:A:413:LEU:HD13	1.77	0.65
1:A:95:ARG:CZ	1:B:26:GLU:HG2	2.26	0.65
1:A:199:GLU:N	1:A:199:GLU:OE1	2.30	0.65
1:A:95:ARG:NE	1:A:262:PRO:O	2.29	0.65
1:A:157:ILE:CG2	1:A:169:LYS:HD2	2.26	0.65
1:A:202:TYR:O	1:A:257:PHE:HD1	1.80	0.65
1:A:220:LEU:HG	1:A:221:PRO:CD	2.27	0.65
1:A:332:ASP:O	1:A:418:ARG:N	2.26	0.65
1:A:420:VAL:CG2	1:A:465:VAL:HB	2.27	0.65
1:A:101:SER:CA	1:A:104:ASN:ND2	2.59	0.65
1:A:150:GLU:OE1	1:A:173:ILE:HD12	1.97	0.65
1:A:377:ASN:ND2	1:A:411:ARG:HG2	2.12	0.65
1:A:200:LEU:HD11	1:A:207:ALA:HB1	1.78	0.64
1:A:516:GLU:OE1	1:A:540:PHE:HD1	1.80	0.64
1:A:371:ASP:O	1:A:416:GLU:HB2	1.97	0.64
1:B:310:GLU:HG2	1:B:311:GLN:N	2.12	0.64
1:A:77:GLU:HG3	1:A:78:PHE:H	1.63	0.64
1:A:282:GLU:OE2	1:A:417:ARG:NH2	2.30	0.64
1:A:292:HIS:CD2	1:A:292:HIS:O	2.50	0.64
1:B:529:GLY:O	1:B:532:PHE:HB2	1.96	0.64
1:A:151:SER:O	1:A:154:MET:HB2	1.97	0.64
1:A:264:PRO:HB3	1:A:287:ILE:HD12	1.80	0.64
1:A:33:GLN:O	1:A:37:GLN:HB2	1.98	0.63
1:B:253:ALA:CB	1:B:367:GLY:O	2.46	0.63
1:B:284:TYR:CE1	1:B:292:HIS:CD2	2.83	0.63
1:A:152:LEU:O	1:A:155:ARG:HB2	1.98	0.63
1:A:229:THR:HB	1:A:233:GLU:HG2	1.78	0.63
1:B:305:LEU:HD13	1:B:305:LEU:N	2.12	0.63
1:B:420:VAL:HG13	1:B:465:VAL:HB	1.79	0.63
1:A:104:ASN:OD1	1:A:122:PHE:O	2.17	0.63
1:A:519:ARG:HD3	1:A:540:PHE:HB2	1.79	0.63
1:B:116:LEU:C	1:B:117:THR:HG22	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:GLY:O	1:A:532:PHE:HB2	1.99	0.63
1:B:108:CYS:CB	1:B:113:HIS:ND1	2.61	0.63
1:A:420:VAL:O	1:A:420:VAL:CG2	2.45	0.62
1:A:489:ASP:CA	1:A:514:PHE:CD1	2.82	0.62
1:B:370:ALA:N	1:B:476:TYR:OH	2.28	0.62
1:A:143:PHE:O	1:A:194:LEU:N	2.31	0.62
1:A:145:PRO:HD2	1:A:193:HIS:HA	1.80	0.62
1:A:438:ILE:O	1:A:536:HIS:HE1	1.83	0.62
1:A:154:MET:O	1:A:158:SER:OG	2.16	0.62
1:A:206:ALA:HB3	5:A:594:HOH:O	1.99	0.62
1:A:309:ASN:N	1:A:309:ASN:ND2	2.43	0.62
1:B:61:VAL:CG2	1:B:62:VAL:N	2.62	0.62
1:B:245:GLU:O	1:B:248:ILE:CG2	2.47	0.62
1:B:338:ILE:HD11	1:B:414:TYR:HD2	1.64	0.62
1:A:54:TYR:O	1:A:58:VAL:HG12	1.99	0.62
1:A:292:HIS:HD2	1:A:296:GLU:HG2	1.63	0.62
1:A:304:TYR:CE2	1:A:328:LEU:CD2	2.82	0.62
1:B:58:VAL:O	1:B:61:VAL:HG22	2.00	0.62
1:A:358:GLN:C	1:A:360:VAL:H	2.06	0.62
1:A:200:LEU:CD2	1:A:201:PHE:N	2.43	0.61
1:B:102:PHE:O	1:B:106:VAL:HG23	2.00	0.61
1:B:124:PHE:HB2	1:B:299:ARG:CD	2.29	0.61
1:A:75:ASP:CB	1:A:77:GLU:HG2	2.27	0.61
1:A:365:ARG:HB3	1:A:369:MET:HB2	1.83	0.61
1:A:422:LEU:HB3	1:A:460:PHE:O	2.01	0.61
1:A:516:GLU:OE1	1:A:540:PHE:CD1	2.53	0.61
1:B:220:LEU:HD12	1:B:221:PRO:CD	2.30	0.61
1:A:170:SER:O	1:A:173:ILE:HG12	2.00	0.61
1:A:509:SER:N	1:A:510:PRO:HD2	2.13	0.61
1:A:240:LEU:HD23	1:A:245:GLU:HG3	1.75	0.61
1:B:124:PHE:HB2	1:B:299:ARG:HG3	1.80	0.61
1:B:253:ALA:HB1	1:B:367:GLY:O	2.00	0.61
1:B:482:MET:HE2	1:B:545:TRP:CZ3	2.31	0.61
1:A:423:ASN:OD1	1:A:461:LYS:HB2	2.00	0.61
1:B:228:GLN:HE21	1:B:232:GLY:HA2	1.64	0.61
1:B:413:LEU:O	1:B:413:LEU:CD2	2.41	0.61
1:A:69:THR:HG22	1:A:73:SER:OG	2.01	0.61
1:A:127:GLN:N	1:A:128:PRO:CD	2.61	0.61
1:B:448:LEU:HD13	1:B:453:ILE:HG22	1.82	0.61
1:A:119:GLU:OE1	1:A:119:GLU:N	2.34	0.61
1:A:133:ARG:O	1:A:133:ARG:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:CYS:SG	1:A:113:HIS:HA	2.40	0.60
1:A:208:TRP:CZ3	1:A:225:PRO:HG3	2.36	0.60
1:B:389:LEU:O	1:B:389:LEU:HG	2.00	0.60
1:B:391:GLU:HA	1:B:394:LEU:HB3	1.83	0.60
1:B:95:ARG:NH2	1:B:262:PRO:O	2.25	0.60
1:B:265:ALA:O	1:B:269:GLU:HB2	2.01	0.60
1:A:86:TYR:O	1:A:90:LEU:CD1	2.50	0.60
1:A:101:SER:HA	1:A:104:ASN:HD21	1.63	0.60
1:A:132:PHE:O	1:A:134:THR:N	2.28	0.60
1:A:264:PRO:O	1:A:268:VAL:HG23	2.01	0.60
1:A:324:LEU:N	1:A:337:VAL:O	2.29	0.60
1:A:420:VAL:HG22	1:A:465:VAL:HB	1.84	0.60
1:A:237:ASP:OD1	1:A:237:ASP:C	2.43	0.60
1:A:266:ALA:O	1:A:269:GLU:HB3	2.02	0.60
1:A:557:VAL:O	1:A:557:VAL:CG1	2.49	0.60
1:A:126:SER:O	1:A:127:GLN:HB3	2.01	0.60
1:A:229:THR:N	1:A:233:GLU:O	2.33	0.60
1:B:315:ALA:HB3	1:B:325:VAL:HG11	1.84	0.60
1:B:514:PHE:HD2	1:B:517:GLU:HB2	1.66	0.60
1:B:270:TRP:HE3	1:B:271:LEU:HG	1.66	0.60
1:A:116:LEU:HD12	1:A:117:THR:H	1.66	0.59
1:A:331:PHE:HD1	1:A:332:ASP:H	1.49	0.59
1:A:463:PHE:HB3	1:A:471:VAL:CG1	2.31	0.59
1:B:525:ASP:CB	1:B:528:ILE:HD12	2.32	0.59
1:A:127:GLN:O	1:A:128:PRO:C	2.42	0.59
1:A:20:GLN:NE2	1:A:20:GLN:C	2.61	0.59
1:A:488:ARG:O	1:A:514:PHE:HE1	1.83	0.59
1:B:108:CYS:CB	1:B:113:HIS:HD1	2.15	0.59
1:A:305:LEU:HD13	1:A:305:LEU:N	2.07	0.59
1:A:351:ALA:HB3	1:A:354:ARG:HG3	1.83	0.59
1:A:357:TYR:CE1	1:A:476:TYR:CD2	2.89	0.59
1:A:86:TYR:O	1:A:90:LEU:HD12	2.03	0.59
1:A:213:LEU:HG	1:A:213:LEU:O	2.01	0.59
1:B:370:ALA:H	1:B:476:TYR:HH	1.51	0.59
1:A:371:ASP:CG	1:A:372:THR:N	2.60	0.59
1:B:124:PHE:CB	1:B:299:ARG:CD	2.80	0.59
1:B:420:VAL:HG21	1:B:425:TRP:HD1	1.67	0.59
1:B:104:ASN:HB2	4:B:1604:AMP:O3'	2.03	0.59
1:A:19:ALA:O	1:A:22:GLY:N	2.36	0.59
1:B:261:ALA:HB2	1:B:267:LEU:HD22	1.84	0.59
1:B:359:LEU:O	1:B:363:HIS:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LEU:HD13	1:A:86:TYR:OH	2.01	0.58
1:A:58:VAL:HG23	1:A:106:VAL:HG22	1.84	0.58
1:A:489:ASP:HB3	1:A:514:PHE:HB3	1.85	0.58
1:B:323:MET:HE1	1:B:477:ASP:OD1	2.03	0.58
1:A:61:VAL:O	1:A:65:LEU:HB2	2.03	0.58
1:A:109:ARG:NH1	1:A:374:GLU:OE1	2.36	0.58
1:A:161:PRO:HB3	1:B:138:PRO:HB3	1.84	0.58
1:A:252:PHE:O	1:A:365:ARG:NH1	2.37	0.58
1:A:301:TYR:HA	1:A:331:PHE:HZ	1.67	0.58
1:B:208:TRP:CZ3	1:B:223:LEU:HD22	2.38	0.58
1:B:403:ASP:C	1:B:404:LEU:HD23	2.28	0.58
1:A:127:GLN:N	1:A:128:PRO:HD2	2.17	0.58
1:A:335:PHE:N	1:A:335:PHE:CD2	2.71	0.58
1:B:220:LEU:CD1	1:B:221:PRO:HD2	2.34	0.58
1:B:310:GLU:CG	1:B:328:LEU:HD23	2.31	0.58
1:A:101:SER:CA	1:A:104:ASN:HD22	2.16	0.58
1:A:245:GLU:O	1:A:249:VAL:HG12	2.03	0.58
1:A:304:TYR:HE2	1:A:328:LEU:CD2	2.15	0.58
1:B:95:ARG:NH2	1:B:262:PRO:CB	2.67	0.58
1:B:327:THR:C	1:B:328:LEU:HD12	2.29	0.58
1:B:442:GLY:O	1:B:446:ARG:HG3	2.04	0.58
1:B:221:PRO:HG3	1:B:274:ILE:O	2.03	0.58
1:B:295:THR:HG22	1:B:296:GLU:N	2.16	0.58
1:B:541:ARG:O	1:B:541:ARG:HG2	2.04	0.58
1:A:39:ASP:O	1:A:42:ALA:HB3	2.04	0.57
1:A:490:ILE:O	1:A:491:PRO:C	2.46	0.57
1:B:32:GLN:HE22	1:B:161:PRO:HB3	1.69	0.57
1:B:253:ALA:HA	1:B:369:MET:O	2.05	0.57
1:B:327:THR:OG1	1:B:334:VAL:HA	2.04	0.57
1:B:450:ALA:HB1	1:B:558:GLU:CB	2.34	0.57
1:A:154:MET:HE1	1:A:169:LYS:HE3	1.87	0.57
1:B:552:ILE:C	1:B:554:GLU:H	2.10	0.57
1:A:340:ASP:OD1	1:A:400:LYS:CG	2.53	0.57
1:A:78:PHE:C	1:A:80:LEU:H	2.11	0.57
1:A:325:VAL:HG11	2:A:1762:ADP:C1'	2.34	0.57
1:A:48:LYS:O	1:A:52:HIS:ND1	2.37	0.57
1:B:78:PHE:O	1:B:82:VAL:HG23	2.04	0.57
1:B:124:PHE:HB3	1:B:299:ARG:HG2	1.82	0.57
1:B:354:ARG:HE	1:B:412:HIS:CD2	2.23	0.57
1:A:215:THR:O	1:A:218:GLY:O	2.23	0.57
1:A:292:HIS:CD2	1:A:296:GLU:CG	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:GLN:HA	1:B:433:GLN:OE1	2.04	0.57
1:A:145:PRO:CD	1:A:193:HIS:HA	2.35	0.57
1:A:449:ALA:CB	1:A:548:LEU:HD13	2.35	0.57
1:A:222:PHE:O	1:A:222:PHE:CD2	2.58	0.56
1:A:200:LEU:HD23	1:A:201:PHE:C	2.29	0.56
1:A:222:PHE:HE2	1:A:224:LEU:HD12	1.69	0.56
1:B:356:CYS:SG	1:B:479:ILE:HG22	2.45	0.56
1:A:23:ARG:HB3	1:A:53:LEU:HD22	1.87	0.56
1:A:200:LEU:CD2	1:A:201:PHE:C	2.78	0.56
1:A:294:LYS:HG3	1:A:373:GLN:HG3	1.87	0.56
1:A:315:ALA:HB3	1:A:325:VAL:HG13	1.87	0.56
1:A:380:LEU:HD13	1:A:410:ILE:HG21	1.86	0.56
1:B:179:HIS:CD2	1:B:241:THR:OG1	2.57	0.56
1:B:334:VAL:HB	1:B:418:ARG:HB3	1.87	0.56
1:A:425:TRP:O	1:A:429:VAL:HG22	2.05	0.56
1:A:568:ARG:CG	1:A:571:VAL:HG12	2.35	0.56
1:A:68:ILE:HG13	1:B:67:CYS:SG	2.45	0.56
1:A:489:ASP:HA	1:A:514:PHE:CE1	2.39	0.56
1:B:9:ILE:HG21	1:B:82:VAL:HG22	1.87	0.56
1:B:93:TYR:HB3	1:B:96:PHE:CB	2.35	0.56
1:A:113:HIS:CB	1:A:376:GLU:HB3	2.35	0.56
1:B:325:VAL:HG22	1:B:334:VAL:HG22	1.87	0.56
1:A:325:VAL:HG13	1:A:325:VAL:O	2.06	0.56
1:A:442:GLY:HA3	1:A:536:HIS:NE2	2.21	0.56
1:A:458:MET:CE	5:A:601:HOH:O	2.50	0.56
1:B:326:PHE:CE2	1:B:337:VAL:HG12	2.36	0.56
1:A:308:CYS:SG	1:A:309:ASN:N	2.78	0.55
1:A:449:ALA:HB1	1:A:548:LEU:HD13	1.88	0.55
1:B:482:MET:CE	1:B:545:TRP:HZ3	2.16	0.55
1:A:299:ARG:O	1:A:303:VAL:HG23	2.06	0.55
1:B:96:PHE:CD1	1:B:96:PHE:C	2.84	0.55
1:B:411:ARG:O	1:B:412:HIS:HB3	2.06	0.55
1:A:423:ASN:OD1	1:A:461:LYS:HB3	2.06	0.55
1:A:488:ARG:NH2	1:A:490:ILE:HB	2.21	0.55
1:B:95:ARG:NH1	5:B:603:HOH:O	2.02	0.55
1:B:149:TRP:HB3	1:B:177:ILE:HD11	1.87	0.55
1:B:318:ILE:HB	1:B:461:LYS:CE	2.37	0.55
1:A:108:CYS:CB	1:A:113:HIS:HA	2.36	0.55
1:B:394:LEU:HA	1:B:401:ILE:HD13	1.88	0.55
1:A:244:ALA:O	1:A:248:ILE:HG12	2.06	0.55
1:B:51:ILE:HD11	1:B:256:TYR:HD2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:TYR:HE2	1:B:116:LEU:HA	1.72	0.55
1:B:171:ARG:O	1:B:175:TYR:HD2	1.90	0.55
1:B:529:GLY:O	1:B:532:PHE:N	2.27	0.55
1:A:23:ARG:HB3	1:A:53:LEU:CD2	2.37	0.55
1:B:441:TYR:O	1:B:444:ALA:HB3	2.06	0.55
1:B:353:VAL:O	1:B:354:ARG:C	2.50	0.55
1:A:209:LEU:HB3	1:A:224:LEU:HB2	1.89	0.55
1:A:250:PHE:HB2	1:A:275:LEU:HD21	1.87	0.55
1:B:372:THR:HG22	1:B:415:ILE:O	2.07	0.55
1:A:153:LEU:HD21	1:A:176:ILE:HG21	1.87	0.55
1:A:201:PHE:O	1:A:208:TRP:HB2	2.07	0.54
1:A:212:LYS:HZ2	1:A:270:TRP:CD1	2.24	0.54
1:A:189:LEU:O	1:A:190:SER:CB	2.55	0.54
1:A:255:SER:CA	1:A:365:ARG:HH21	2.18	0.54
1:B:134:THR:HG22	1:B:134:THR:O	2.06	0.54
1:B:312:PHE:CD2	1:B:384:HIS:HB3	2.42	0.54
1:A:95:ARG:NH2	1:B:26:GLU:CD	2.65	0.54
1:B:338:ILE:HG22	1:B:339:LYS:O	2.08	0.54
1:B:61:VAL:CG2	1:B:62:VAL:H	2.20	0.54
1:B:294:LYS:NZ	4:B:1604:AMP:O3P	2.30	0.54
1:B:324:LEU:HD13	1:B:393:LEU:HD12	1.89	0.54
1:A:76:ALA:O	1:A:77:GLU:C	2.50	0.54
1:A:25:LEU:O	1:A:29:SER:HB3	2.06	0.54
1:A:408:ILE:HG12	1:A:408:ILE:O	2.05	0.54
1:B:231:ASP:OD1	1:B:231:ASP:N	2.29	0.54
1:A:221:PRO:HB3	1:A:274:ILE:HG23	1.90	0.54
1:A:442:GLY:HA3	1:A:536:HIS:CE1	2.43	0.54
1:A:128:PRO:CB	1:A:129:GLU:CA	2.38	0.54
1:B:195:GLN:O	1:B:212:LYS:N	2.33	0.54
1:B:255:SER:OG	1:B:364:ASP:OD1	2.26	0.54
1:A:97:GLU:HB2	1:A:292:HIS:CE1	2.42	0.54
1:A:170:SER:O	1:A:173:ILE:CG1	2.56	0.54
1:A:456:GLY:HA3	1:A:478:GLU:O	2.08	0.54
1:A:359:LEU:HD23	1:A:359:LEU:O	2.08	0.54
1:A:372:THR:HA	1:A:415:ILE:O	2.08	0.54
1:B:237:ASP:OD2	1:B:563:TYR:OH	2.22	0.54
1:B:275:LEU:C	1:B:277:GLY:N	2.65	0.54
1:B:290:GLN:HA	1:B:293:ALA:HB3	1.90	0.54
1:B:462:ASN:HB3	1:B:475:ASP:HB2	1.90	0.54
1:B:118:PRO:CD	1:B:119:GLU:N	2.71	0.53
1:B:538:ASP:OD1	1:B:538:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:VAL:O	1:B:357:TYR:HB2	2.09	0.53
1:B:375:PHE:HE2	1:B:415:ILE:HD12	1.73	0.53
1:A:366:VAL:HG12	1:A:366:VAL:O	2.09	0.53
1:B:280:THR:O	1:B:284:TYR:HD2	1.90	0.53
1:B:287:ILE:O	1:B:287:ILE:HG22	2.08	0.53
1:B:465:VAL:HA	1:B:470:ARG:O	2.08	0.53
1:A:490:ILE:O	1:A:491:PRO:O	2.25	0.53
1:A:96:PHE:CZ	1:A:128:PRO:CG	2.92	0.53
1:A:194:LEU:CD2	1:A:195:GLN:N	2.72	0.53
1:A:292:HIS:HD2	1:A:296:GLU:CG	2.21	0.53
1:A:449:ALA:O	1:A:451:ALA:O	2.25	0.53
1:A:457:ASP:OD1	1:A:457:ASP:C	2.52	0.53
1:A:483:THR:HG23	1:A:553:ARG:HD3	1.91	0.53
1:B:48:LYS:NZ	5:B:610:HOH:O	2.30	0.53
1:B:561:TYR:HB3	1:B:563:TYR:CE1	2.43	0.53
1:A:358:GLN:O	1:A:361:LYS:N	2.38	0.53
1:A:488:ARG:HB2	1:A:546:ARG:HH22	1.73	0.53
1:A:489:ASP:HB3	1:A:514:PHE:CB	2.39	0.53
1:B:427:GLU:O	1:B:429:VAL:N	2.39	0.53
1:B:556:HIS:CE1	5:B:579:HOH:O	2.60	0.53
1:B:79:LEU:HD12	1:B:120:ARG:HB3	1.90	0.53
1:B:313:ILE:O	1:B:327:THR:N	2.40	0.53
1:A:194:LEU:HD23	1:A:195:GLN:H	1.73	0.53
1:A:200:LEU:CD2	1:A:200:LEU:O	2.55	0.53
1:B:294:LYS:HG3	1:B:373:GLN:OE1	2.09	0.53
1:A:334:VAL:O	1:A:415:ILE:HA	2.08	0.52
1:B:85:HIS:O	1:B:88:ARG:HG2	2.08	0.52
1:B:127:GLN:CB	1:B:128:PRO:HD3	2.26	0.52
1:B:251:GLY:O	1:B:254:ARG:HB2	2.09	0.52
1:A:317:GLY:HA2	1:A:424:ILE:HD11	1.91	0.52
1:A:359:LEU:HD21	1:A:481:TYR:CE1	2.44	0.52
1:B:222:PHE:C	1:B:222:PHE:CD2	2.87	0.52
1:B:338:ILE:HG21	1:B:353:VAL:HG11	1.90	0.52
1:A:40:TRP:HD1	1:A:43:VAL:HB	1.74	0.52
1:B:177:ILE:O	1:B:181:THR:N	2.43	0.52
1:B:448:LEU:HD12	1:B:455:PRO:HG3	1.91	0.52
1:A:264:PRO:CB	1:A:287:ILE:HD12	2.40	0.52
1:B:63:GLU:O	1:B:67:CYS:HB2	2.10	0.52
1:B:168:ASN:C	1:B:170:SER:H	2.16	0.52
1:B:278:LYS:HB2	1:B:282:GLU:OE2	2.10	0.52
1:B:286:ALA:O	1:B:287:ILE:HD12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:THR:C	1:B:217:SER:N	2.66	0.52
1:A:95:ARG:NH2	1:B:26:GLU:CG	2.72	0.52
1:A:445:ILE:HG22	1:A:445:ILE:O	2.10	0.52
1:B:186:PRO:HA	1:B:189:LEU:HD22	1.90	0.52
1:B:80:LEU:HD11	1:B:119:GLU:O	2.08	0.52
1:B:101:SER:HA	1:B:104:ASN:ND2	2.25	0.52
1:B:338:ILE:HG12	1:B:353:VAL:CG2	2.33	0.52
1:A:33:GLN:O	1:A:37:GLN:N	2.40	0.52
1:B:124:PHE:HB3	1:B:299:ARG:HD3	1.90	0.52
1:B:176:ILE:HD11	1:B:236:ILE:HD12	1.92	0.52
1:B:482:MET:CE	1:B:545:TRP:CZ3	2.92	0.52
1:B:569:PHE:O	1:B:573:TYR:O	2.28	0.52
1:A:336:LYS:HD2	1:A:416:GLU:OE1	2.09	0.52
1:A:358:GLN:HA	1:A:361:LYS:HB2	1.92	0.51
1:B:438:ILE:HB	1:B:532:PHE:CE2	2.45	0.51
1:A:127:GLN:O	1:A:128:PRO:O	2.29	0.51
1:A:380:LEU:HD13	1:A:410:ILE:CG2	2.40	0.51
1:B:222:PHE:CD2	1:B:222:PHE:O	2.63	0.51
1:B:514:PHE:CD2	1:B:517:GLU:HB2	2.45	0.51
1:A:194:LEU:CD2	1:A:195:GLN:H	2.23	0.51
1:A:237:ASP:OD1	1:A:238:THR:N	2.43	0.51
1:B:204:ASN:ND2	1:B:560:VAL:HG11	2.24	0.51
1:B:564:ARG:HG3	1:B:564:ARG:NH2	2.24	0.51
1:A:194:LEU:HD22	1:A:195:GLN:N	2.25	0.51
1:B:40:TRP:HD1	1:B:43:VAL:HG21	1.76	0.51
1:B:430:GLU:N	1:B:430:GLU:OE2	2.44	0.51
1:A:57:HIS:O	1:A:61:VAL:CG1	2.58	0.51
1:A:74:THR:HA	1:A:78:PHE:HE1	1.76	0.51
1:A:132:PHE:C	1:A:134:THR:N	2.66	0.51
1:B:189:LEU:C	1:B:189:LEU:HD23	2.36	0.51
1:B:374:GLU:HB2	1:B:414:TYR:CE1	2.46	0.51
1:A:462:ASN:HB3	1:A:475:ASP:HB2	1.93	0.51
1:B:62:VAL:HG21	1:B:109:ARG:HB3	1.93	0.51
1:B:154:MET:HG3	1:B:173:ILE:HG21	1.92	0.51
1:B:515:PRO:HB3	1:B:545:TRP:NE1	2.25	0.51
1:B:569:PHE:O	1:B:573:TYR:HB2	2.11	0.51
1:A:33:GLN:HE22	1:B:134:THR:HG23	1.75	0.51
1:A:81:ARG:O	1:A:85:HIS:CD2	2.63	0.51
1:A:138:PRO:HB2	1:A:140:ALA:O	2.11	0.51
1:B:368:ARG:C	1:B:369:MET:HG2	2.35	0.51
1:A:32:GLN:OE1	1:B:138:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ARG:CG	1:B:81:ARG:NH2	2.66	0.51
1:B:116:LEU:O	1:B:117:THR:HG22	2.11	0.51
1:B:312:PHE:HD2	1:B:384:HIS:HB3	1.74	0.51
1:B:422:LEU:O	1:B:425:TRP:N	2.44	0.51
1:A:356:CYS:O	1:A:360:VAL:HG23	2.11	0.51
1:B:280:THR:HG22	1:B:284:TYR:CE2	2.46	0.51
1:B:304:TYR:CD2	1:B:304:TYR:C	2.89	0.51
1:B:327:THR:HG23	1:B:328:LEU:H	1.73	0.51
1:A:114:ARG:HD3	1:A:114:ARG:C	2.36	0.51
1:A:212:LYS:HZ2	1:A:270:TRP:NE1	2.09	0.51
1:A:268:VAL:HG13	1:A:283:LEU:HB2	1.93	0.51
1:A:336:LYS:HB2	1:A:414:TYR:HB2	1.93	0.51
1:B:95:ARG:HD3	1:B:262:PRO:O	2.11	0.51
1:B:382:LYS:HG3	1:B:408:ILE:HG12	1.92	0.51
1:B:450:ALA:HB1	1:B:558:GLU:CD	2.36	0.51
1:B:559:ASP:HB3	1:B:561:TYR:CE2	2.46	0.51
1:A:53:LEU:HA	1:A:56:HIS:HB3	1.93	0.50
1:A:155:ARG:C	1:A:159:ASP:OD2	2.52	0.50
1:A:260:TYR:O	1:A:260:TYR:CD2	2.64	0.50
1:A:101:SER:C	1:A:104:ASN:HD22	2.18	0.50
1:A:134:THR:O	1:A:134:THR:OG1	2.29	0.50
1:B:54:TYR:CG	1:B:291:LYS:HD3	2.46	0.50
1:A:189:LEU:O	1:A:190:SER:HB2	2.10	0.50
1:A:439:GLU:HG3	1:A:535:MET:HG3	1.94	0.50
1:B:334:VAL:CG1	1:B:416:GLU:HG3	2.41	0.50
1:B:518:PHE:O	1:B:522:LEU:HB2	2.11	0.50
1:B:525:ASP:HB3	1:B:528:ILE:CD1	2.40	0.50
1:B:315:ALA:HB3	1:B:325:VAL:CG1	2.41	0.50
1:A:55:ASP:HA	1:A:58:VAL:HG13	1.93	0.50
1:A:149:TRP:CD1	1:A:189:LEU:HG	2.47	0.50
1:B:29:SER:HB3	1:B:260:TYR:HD1	1.75	0.50
1:B:241:THR:N	1:B:245:GLU:OE1	2.37	0.50
1:B:239:CYS:HB2	1:B:569:PHE:HZ	1.77	0.50
1:B:318:ILE:HB	1:B:461:LYS:HE2	1.94	0.50
1:B:368:ARG:O	1:B:473:PHE:HB3	2.11	0.50
1:A:414:TYR:O	1:A:415:ILE:HD12	2.11	0.50
1:B:61:VAL:HG23	1:B:62:VAL:H	1.73	0.50
1:B:194:LEU:HD12	1:B:213:LEU:HA	1.94	0.50
1:A:160:LEU:C	1:A:162:LEU:H	2.19	0.50
1:B:21:TYR:O	1:B:24:PHE:CB	2.59	0.50
1:A:20:GLN:NE2	1:A:20:GLN:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASN:OD1	1:A:198:ASN:O	2.30	0.49
1:A:222:PHE:CD2	1:A:222:PHE:C	2.90	0.49
1:A:375:PHE:O	1:A:412:HIS:HA	2.12	0.49
1:A:519:ARG:HD3	1:A:540:PHE:CB	2.42	0.49
1:B:448:LEU:HD13	1:B:453:ILE:HG21	1.94	0.49
1:A:212:LYS:HZ2	1:A:270:TRP:CG	2.30	0.49
1:B:176:ILE:HD11	1:B:236:ILE:CD1	2.41	0.49
1:B:287:ILE:O	1:B:287:ILE:CG2	2.60	0.49
1:B:366:VAL:CG1	1:B:366:VAL:O	2.59	0.49
1:A:382:LYS:CB	1:A:406:GLU:O	2.58	0.49
1:B:196:VAL:HG13	1:B:209:LEU:HD21	1.93	0.49
1:B:339:LYS:HD3	1:B:342:PHE:HA	1.93	0.49
1:B:376:GLU:HA	1:B:412:HIS:N	2.25	0.49
1:A:107:TYR:CZ	1:A:120:ARG:HG3	2.48	0.49
1:A:328:LEU:CD1	1:A:329:PRO:HD2	2.31	0.49
1:B:310:GLU:OE2	1:B:384:HIS:CE1	2.66	0.49
1:B:476:TYR:HB3	1:B:479:ILE:HD12	1.94	0.49
1:A:157:ILE:HG22	1:A:169:LYS:HD2	1.92	0.49
1:A:197:ALA:HB3	1:A:210:VAL:CG1	2.43	0.49
1:A:411:ARG:O	1:A:412:HIS:HD2	1.93	0.49
1:B:223:LEU:HD13	1:B:249:VAL:HG11	1.94	0.49
1:B:481:TYR:C	1:B:483:THR:H	2.21	0.49
1:A:48:LYS:O	1:A:52:HIS:CE1	2.65	0.49
1:A:470:ARG:HB3	1:A:470:ARG:CZ	2.43	0.49
1:A:516:GLU:C	1:A:518:PHE:N	2.69	0.49
1:A:525:ASP:CB	1:A:528:ILE:HG12	2.39	0.49
1:B:382:LYS:NZ	1:B:403:ASP:CG	2.54	0.49
1:A:40:TRP:CD1	1:A:43:VAL:HB	2.48	0.49
1:A:305:LEU:HD23	1:A:381:GLU:OE2	2.12	0.49
1:B:322:VAL:HG23	1:B:323:MET:N	2.26	0.49
1:B:387:PRO:HA	1:B:390:MET:HB3	1.92	0.49
1:A:7:LEU:O	1:A:11:GLN:HB2	2.13	0.49
1:A:103:PHE:C	1:A:103:PHE:CD2	2.91	0.49
1:A:125:SER:HB2	1:A:129:GLU:CG	2.40	0.49
1:A:249:VAL:HG13	1:A:250:PHE:HD2	1.78	0.49
1:A:339:LYS:HD2	1:A:396:GLU:OE1	2.12	0.49
1:A:355:ALA:O	1:A:359:LEU:HB2	2.13	0.49
1:B:124:PHE:CD2	1:B:299:ARG:HD3	2.47	0.49
1:B:539:LEU:O	1:B:545:TRP:NE1	2.43	0.49
1:A:453:ILE:HG23	1:A:479:ILE:HD12	1.95	0.49
1:A:461:LYS:H	1:A:461:LYS:CD	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:HIS:H	1:A:165:HIS:CD2	2.30	0.48
1:B:304:TYR:HB3	1:B:305:LEU:HD13	1.95	0.48
1:A:333:ARG:HA	1:A:418:ARG:H	1.79	0.48
1:A:338:ILE:H	1:A:338:ILE:CD1	2.24	0.48
1:A:441:TYR:O	1:A:444:ALA:HB3	2.13	0.48
1:B:95:ARG:HH22	1:B:262:PRO:CB	2.20	0.48
1:B:121:LEU:C	1:B:121:LEU:HD12	2.38	0.48
1:B:328:LEU:HB3	1:B:329:PRO:HD2	1.96	0.48
1:A:240:LEU:HD22	1:A:245:GLU:CB	2.43	0.48
1:A:338:ILE:N	1:A:338:ILE:CD1	2.67	0.48
1:B:338:ILE:HD11	1:B:414:TYR:CD2	2.46	0.48
1:B:565:ARG:C	1:B:567:GLN:N	2.71	0.48
1:A:222:PHE:HE2	1:A:224:LEU:CD1	2.26	0.48
1:A:308:CYS:O	1:A:309:ASN:ND2	2.45	0.48
1:A:336:LYS:N	1:A:414:TYR:O	2.31	0.48
1:A:368:ARG:HH22	1:A:440:GLU:HG3	1.78	0.48
1:B:47:MET:HG3	1:B:47:MET:O	2.14	0.48
1:B:340:ASP:OD1	1:B:340:ASP:N	2.40	0.48
1:A:68:ILE:HG22	1:A:68:ILE:O	2.14	0.48
1:A:356:CYS:HB3	1:A:476:TYR:O	2.10	0.48
1:B:85:HIS:HA	1:B:88:ARG:HD3	1.96	0.48
1:A:116:LEU:CD1	1:A:117:THR:H	2.27	0.48
1:A:302:LEU:O	1:A:306:GLN:HB2	2.14	0.48
1:B:430:GLU:N	1:B:430:GLU:CD	2.72	0.48
1:B:438:ILE:CD1	1:B:531:LEU:HB3	2.41	0.48
1:B:116:LEU:O	1:B:117:THR:CB	2.56	0.48
1:B:251:GLY:O	1:B:254:ARG:CG	2.62	0.48
1:A:241:THR:HG22	1:A:241:THR:O	2.13	0.48
1:B:47:MET:HE1	1:B:255:SER:HB3	1.96	0.48
1:B:304:TYR:CE2	1:B:305:LEU:HD12	2.45	0.48
1:A:189:LEU:HD21	1:A:190:SER:OG	2.13	0.48
1:A:335:PHE:CB	1:A:413:LEU:HD11	2.37	0.48
1:B:203:ARG:NH1	1:B:255:SER:O	2.47	0.48
1:B:538:ASP:HA	1:B:541:ARG:HD3	1.95	0.48
1:A:78:PHE:C	1:A:80:LEU:N	2.68	0.47
1:A:281:ALA:HB2	1:A:296:GLU:HB3	1.95	0.47
1:A:452:ASN:OD1	1:A:552:ILE:CG2	2.60	0.47
1:A:450:ALA:O	1:A:557:VAL:CG2	2.63	0.47
1:B:7:LEU:HD22	1:B:8:LEU:N	2.28	0.47
1:B:16:GLY:O	1:B:20:GLN:HB2	2.14	0.47
1:B:108:CYS:HB3	1:B:113:HIS:HD1	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:TYR:C	1:B:441:TYR:CD2	2.91	0.47
1:A:25:LEU:HB2	1:A:260:TYR:CE1	2.49	0.47
1:A:447:GLN:NE2	5:A:580:HOH:O	2.47	0.47
1:A:535:MET:HE3	1:A:535:MET:O	2.14	0.47
1:B:327:THR:HG21	1:B:418:ARG:HD3	1.96	0.47
1:A:97:GLU:HG2	1:A:98:ILE:N	2.30	0.47
1:B:375:PHE:CE2	1:B:415:ILE:HD12	2.49	0.47
1:A:25:LEU:HD13	5:B:603:HOH:O	2.14	0.47
1:A:305:LEU:HD22	1:A:306:GLN:N	2.29	0.47
1:B:101:SER:C	1:B:104:ASN:HD22	2.22	0.47
1:B:122:PHE:HB3	1:B:127:GLN:HB2	1.96	0.47
1:B:145:PRO:HB3	1:B:149:TRP:CD1	2.49	0.47
1:B:259:VAL:HG11	1:B:267:LEU:HD21	1.95	0.47
1:B:420:VAL:CG2	1:B:425:TRP:HD1	2.28	0.47
1:A:100:GLU:O	1:A:103:PHE:HB3	2.15	0.47
1:A:112:ASP:O	1:A:113:HIS:C	2.57	0.47
1:A:156:VAL:O	1:A:160:LEU:HG	2.13	0.47
1:A:255:SER:CA	1:A:365:ARG:NH2	2.76	0.47
1:A:460:PHE:HZ	1:A:522:LEU:O	1.98	0.47
1:A:65:LEU:HD22	1:A:110:LEU:HD11	1.97	0.47
1:A:189:LEU:HD23	1:A:190:SER:CB	2.44	0.47
1:A:462:ASN:ND2	1:A:475:ASP:OD2	2.48	0.47
1:A:488:ARG:HD2	1:A:546:ARG:HH22	1.79	0.47
1:A:544:TYR:CE2	1:A:548:LEU:HD11	2.49	0.47
1:B:90:LEU:N	1:B:91:PRO:CD	2.74	0.47
1:B:259:VAL:CG1	1:B:267:LEU:HD21	2.45	0.47
1:B:290:GLN:O	1:B:294:LYS:N	2.41	0.47
1:B:378:PHE:HE2	1:B:380:LEU:HD21	1.80	0.47
1:B:419:MET:HE1	1:B:472:VAL:HG21	1.96	0.47
1:B:422:LEU:O	1:B:423:ASN:C	2.57	0.47
1:B:90:LEU:HD21	1:B:99:ALA:CB	2.45	0.47
1:B:539:LEU:O	1:B:539:LEU:HD23	2.15	0.47
1:A:208:TRP:NE1	5:A:594:HOH:O	2.40	0.47
1:A:304:TYR:CD2	1:A:328:LEU:HD23	2.49	0.47
1:B:58:VAL:HG23	1:B:59:GLY:N	2.30	0.47
1:A:32:GLN:NE2	1:B:138:PRO:HD3	2.30	0.47
1:A:557:VAL:O	1:A:557:VAL:HG12	2.15	0.47
1:A:326:PHE:HE2	1:A:337:VAL:HG21	1.80	0.46
1:A:422:LEU:HD13	1:A:471:VAL:HG13	1.97	0.46
1:B:137:ARG:CB	1:B:138:PRO:CD	2.89	0.46
1:B:203:ARG:HH22	1:B:254:ARG:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ALA:HA	1:B:249:VAL:CG1	2.45	0.46
1:B:376:GLU:CA	1:B:412:HIS:H	2.24	0.46
1:B:380:LEU:CD1	1:B:410:ILE:HD11	2.45	0.46
1:A:84:GLU:HG3	1:A:85:HIS:N	2.27	0.46
1:A:145:PRO:HB3	1:A:148:GLY:HA2	1.96	0.46
1:A:430:GLU:HG3	1:A:431:GLY:N	2.30	0.46
1:A:564:ARG:C	1:A:566:ARG:H	2.23	0.46
1:B:257:PHE:CB	1:B:286:ALA:O	2.46	0.46
1:B:285:MET:HE2	1:B:290:GLN:HG3	1.98	0.46
1:A:5:LEU:O	1:A:9:ILE:HG13	2.16	0.46
1:A:86:TYR:CD2	1:A:90:LEU:HD11	2.50	0.46
1:A:480:CYS:HB2	1:A:484:GLU:OE1	2.16	0.46
1:B:173:ILE:N	5:B:601:HOH:O	2.48	0.46
1:B:271:LEU:O	1:B:274:ILE:HG23	2.14	0.46
1:B:295:THR:O	1:B:298:TYR:N	2.46	0.46
1:A:228:GLN:HG2	1:A:229:THR:N	2.29	0.46
1:A:441:TYR:OH	1:A:458:MET:O	2.30	0.46
1:A:448:LEU:O	1:A:451:ALA:O	2.32	0.46
1:A:163:ARG:HA	1:A:163:ARG:HD2	1.66	0.46
1:A:304:TYR:CD2	1:A:328:LEU:CD2	2.98	0.46
1:B:334:VAL:HB	1:B:418:ARG:CB	2.45	0.46
1:A:412:HIS:CG	1:A:412:HIS:O	2.69	0.46
1:A:458:MET:HB2	5:A:601:HOH:O	2.14	0.46
1:B:149:TRP:HH2	1:B:194:LEU:HD13	1.80	0.46
1:B:318:ILE:O	1:B:319:ARG:C	2.59	0.46
1:B:419:MET:HE3	1:B:419:MET:HB2	1.80	0.46
1:A:151:SER:O	1:A:154:MET:CB	2.62	0.46
1:A:438:ILE:CD1	1:A:531:LEU:HD23	2.45	0.46
1:B:204:ASN:HD22	1:B:560:VAL:CG1	2.28	0.46
1:B:290:GLN:O	1:B:293:ALA:HB3	2.15	0.46
1:A:365:ARG:O	1:A:366:VAL:HB	2.15	0.46
1:A:401:ILE:HA	1:A:409:VAL:O	2.15	0.46
1:A:552:ILE:HA	1:A:556:HIS:O	2.16	0.46
1:B:78:PHE:HD1	1:B:81:ARG:NH2	2.13	0.46
1:B:402:THR:O	1:B:408:ILE:HG22	2.16	0.46
1:A:208:TRP:CE3	1:A:225:PRO:HG3	2.51	0.46
1:B:72:GLN:H	1:B:72:GLN:HG3	1.34	0.46
1:B:173:ILE:HG13	1:B:174:HIS:N	2.31	0.46
1:B:334:VAL:HG12	1:B:416:GLU:HG3	1.96	0.46
1:A:86:TYR:O	1:A:90:LEU:HD11	2.16	0.46
1:B:168:ASN:C	1:B:170:SER:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ARG:HD2	1:B:299:ARG:HA	1.32	0.46
1:B:434:LEU:O	1:B:438:ILE:CG2	2.33	0.46
1:B:450:ALA:HB1	1:B:558:GLU:HB2	1.98	0.46
1:B:525:ASP:CG	1:B:528:ILE:HD12	2.40	0.46
1:A:228:GLN:OE1	1:A:231:ASP:HA	2.16	0.45
1:A:481:TYR:HB2	1:A:484:GLU:HG3	1.97	0.45
1:B:458:MET:O	1:B:458:MET:HG3	2.16	0.45
1:B:565:ARG:C	1:B:567:GLN:H	2.24	0.45
1:B:33:GLN:O	1:B:33:GLN:HG3	2.16	0.45
1:B:301:TYR:O	1:B:305:LEU:HD22	2.15	0.45
1:B:323:MET:CG	1:B:338:ILE:HA	2.44	0.45
1:A:305:LEU:C	1:A:307:GLY:H	2.24	0.45
1:A:488:ARG:HB2	1:A:546:ARG:NH2	2.30	0.45
1:B:376:GLU:OE2	1:B:411:ARG:NH2	2.48	0.45
1:A:153:LEU:O	1:A:156:VAL:HG22	2.16	0.45
1:A:227:HIS:O	1:A:234:LEU:CB	2.62	0.45
1:A:337:VAL:HG22	1:A:413:LEU:CD1	2.45	0.45
1:B:66:ARG:O	1:B:69:THR:O	2.33	0.45
1:A:90:LEU:N	1:A:91:PRO:CD	2.78	0.45
1:A:245:GLU:OE1	1:A:245:GLU:HA	2.17	0.45
1:A:464:GLY:O	1:A:471:VAL:HA	2.16	0.45
1:A:474:TYR:CD1	1:A:474:TYR:C	2.95	0.45
1:A:568:ARG:HG3	1:A:571:VAL:HG12	1.98	0.45
1:A:564:ARG:C	1:A:566:ARG:N	2.75	0.45
1:B:75:ASP:O	1:B:79:LEU:HB2	2.16	0.45
1:B:312:PHE:N	1:B:384:HIS:O	2.38	0.45
1:A:57:HIS:O	1:A:61:VAL:HG13	2.17	0.45
1:A:366:VAL:O	1:A:366:VAL:CG1	2.64	0.45
1:A:516:GLU:O	1:A:517:GLU:C	2.60	0.45
1:B:37:GLN:O	1:B:38:ALA:HB3	2.17	0.45
1:B:125:SER:HA	1:B:296:GLU:CG	2.47	0.45
1:B:274:ILE:CG1	1:B:275:LEU:H	2.25	0.45
1:A:173:ILE:HG13	1:A:174:HIS:N	2.32	0.45
1:B:310:GLU:OE2	1:B:384:HIS:ND1	2.49	0.45
1:A:13:ILE:HA	1:A:61:VAL:HG21	1.98	0.45
1:A:47:MET:O	1:A:50:ARG:N	2.48	0.45
1:A:203:ARG:HB2	1:A:257:PHE:CE1	2.52	0.45
1:A:357:TYR:CD1	1:A:476:TYR:HD2	2.35	0.45
1:A:430:GLU:HG3	1:A:431:GLY:H	1.82	0.45
1:B:126:SER:O	1:B:127:GLN:C	2.58	0.45
1:A:84:GLU:O	1:A:85:HIS:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:SER:O	1:A:127:GLN:CB	2.63	0.45
1:A:477:ASP:C	1:A:479:ILE:H	2.24	0.45
1:B:466:THR:CG2	1:B:467:ARG:N	2.79	0.45
1:B:420:VAL:O	1:B:465:VAL:N	2.40	0.44
1:A:36:GLU:HA	1:A:164:LEU:HD11	1.98	0.44
1:A:296:GLU:O	1:A:300:GLU:HG3	2.17	0.44
1:A:296:GLU:O	1:A:297:SER:C	2.60	0.44
1:A:47:MET:CG	1:A:48:LYS:N	2.77	0.44
1:A:234:LEU:O	1:A:234:LEU:HD22	2.16	0.44
1:A:371:ASP:OD2	1:A:372:THR:N	2.51	0.44
1:B:162:LEU:H	1:B:162:LEU:HD22	1.81	0.44
1:B:226:ILE:CG2	1:B:234:LEU:HD22	2.47	0.44
1:B:544:TYR:O	1:B:548:LEU:CB	2.64	0.44
1:A:153:LEU:HD11	1:A:224:LEU:HD11	2.00	0.44
1:A:301:TYR:HA	1:A:331:PHE:CZ	2.51	0.44
1:A:368:ARG:HB2	1:A:448:LEU:HD13	2.00	0.44
1:B:196:VAL:CG1	1:B:209:LEU:HD21	2.48	0.44
1:B:338:ILE:CG1	1:B:353:VAL:HG21	2.35	0.44
1:A:139:LEU:O	1:A:139:LEU:HD23	2.18	0.44
1:A:204:ASN:C	1:A:206:ALA:H	2.24	0.44
1:A:358:GLN:C	1:A:360:VAL:N	2.72	0.44
1:A:100:GLU:O	1:A:104:ASN:ND2	2.51	0.44
1:A:116:LEU:HD12	1:A:117:THR:N	2.32	0.44
1:A:135:ILE:HG22	1:A:137:ARG:O	2.16	0.44
1:A:255:SER:N	1:A:365:ARG:NH2	2.66	0.44
1:A:323:MET:HE2	1:A:336:LYS:HB3	1.99	0.44
1:B:87:THR:HG22	1:B:122:PHE:HE1	1.80	0.44
1:B:89:LEU:C	1:B:91:PRO:CD	2.84	0.44
1:B:286:ALA:C	1:B:287:ILE:CD1	2.91	0.44
1:B:298:TYR:HA	1:B:301:TYR:HB3	1.99	0.44
1:B:565:ARG:O	1:B:567:GLN:N	2.51	0.44
1:A:127:GLN:O	1:A:127:GLN:HG3	2.17	0.44
1:B:152:LEU:N	1:B:152:LEU:CD2	2.79	0.44
1:B:375:PHE:O	1:B:413:LEU:N	2.50	0.44
1:B:387:PRO:HA	1:B:390:MET:H	1.83	0.44
1:A:17:PHE:CG	1:A:18:ASP:N	2.85	0.44
1:A:153:LEU:HD22	1:A:176:ILE:HG21	1.99	0.44
1:A:474:TYR:OH	2:A:1762:ADP:H2'	2.18	0.44
1:A:516:GLU:CD	1:A:519:ARG:HG3	2.42	0.44
1:B:80:LEU:CD1	1:B:119:GLU:O	2.66	0.44
1:B:164:LEU:CD1	1:B:228:GLN:HE22	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLN:HE21	1:B:290:GLN:HB3	1.46	0.44
1:A:394:LEU:HD23	1:A:401:ILE:HD11	2.00	0.44
1:B:32:GLN:O	1:B:36:GLU:HB2	2.18	0.44
1:B:152:LEU:HD22	1:B:152:LEU:H	1.82	0.44
1:B:549:GLN:C	1:B:551:ARG:N	2.74	0.44
1:B:564:ARG:HH21	1:B:564:ARG:CG	2.25	0.44
1:B:5:LEU:HB2	1:B:78:PHE:CZ	2.53	0.43
1:B:454:PHE:HA	1:B:455:PRO:HD3	1.87	0.43
1:A:23:ARG:HE	1:A:53:LEU:HD11	1.83	0.43
1:A:255:SER:N	1:A:365:ARG:HH21	2.17	0.43
1:A:309:ASN:HA	1:A:310:GLU:HA	1.86	0.43
1:B:297:SER:HA	1:B:300:GLU:HG3	2.01	0.43
1:B:370:ALA:N	1:B:476:TYR:HH	2.14	0.43
1:A:23:ARG:CD	1:A:53:LEU:HD21	2.48	0.43
1:A:567:GLN:O	1:A:568:ARG:C	2.61	0.43
1:B:5:LEU:HA	1:B:8:LEU:HB3	2.00	0.43
1:B:246:ALA:HA	1:B:249:VAL:HG13	2.00	0.43
1:B:274:ILE:CG1	1:B:275:LEU:N	2.80	0.43
1:A:20:GLN:C	1:A:20:GLN:CD	2.86	0.43
1:B:305:LEU:CD1	1:B:305:LEU:N	2.80	0.43
1:A:3:ARG:C	1:A:5:LEU:H	2.27	0.43
1:A:544:TYR:CD2	1:A:544:TYR:C	2.96	0.43
1:B:288:GLY:O	1:B:290:GLN:N	2.42	0.43
1:B:552:ILE:C	1:B:554:GLU:N	2.75	0.43
1:A:172:ASP:HA	1:A:175:TYR:HD2	1.84	0.43
1:A:256:TYR:HB3	1:A:286:ALA:O	2.19	0.43
1:A:432:GLN:HB3	5:A:607:HOH:O	2.18	0.43
1:A:513:VAL:O	1:A:515:PRO:HD3	2.19	0.43
1:B:438:ILE:HB	1:B:532:PHE:CZ	2.53	0.43
1:A:18:ASP:HB3	1:B:19:ALA:HA	1.99	0.43
1:A:81:ARG:O	1:A:85:HIS:HB2	2.19	0.43
1:A:371:ASP:OD2	1:A:372:THR:O	2.36	0.43
1:B:204:ASN:ND2	1:B:560:VAL:CG1	2.82	0.43
1:A:32:GLN:HE22	1:B:138:PRO:HD3	1.83	0.43
1:A:113:HIS:CG	1:A:376:GLU:HB3	2.53	0.43
1:A:490:ILE:HG23	1:A:491:PRO:HD3	2.00	0.43
1:B:121:LEU:C	1:B:121:LEU:CD1	2.91	0.43
1:B:285:MET:C	1:B:287:ILE:H	2.26	0.43
1:B:434:LEU:HD11	1:B:528:ILE:HG23	2.00	0.43
1:B:448:LEU:HD11	1:B:473:PHE:CD2	2.53	0.43
1:A:116:LEU:O	1:A:120:ARG:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:HIS:CE1	1:A:214:ILE:HG21	2.50	0.43
1:A:253:ALA:O	1:A:367:GLY:N	2.50	0.43
1:A:385:ILE:HG22	1:A:386:SER:O	2.19	0.43
1:B:49:ASN:O	1:B:52:HIS:HB2	2.19	0.43
1:B:123:ILE:O	1:B:123:ILE:HG23	2.19	0.43
1:A:170:SER:HA	1:A:173:ILE:HG12	1.99	0.43
1:A:202:TYR:O	1:A:257:PHE:CD1	2.67	0.43
1:A:301:TYR:HD1	1:A:331:PHE:HE2	1.67	0.43
1:B:382:LYS:CE	1:B:403:ASP:OD1	2.64	0.43
1:B:564:ARG:NH2	1:B:564:ARG:CG	2.82	0.43
1:A:23:ARG:HD3	1:A:53:LEU:HD21	2.01	0.42
1:A:139:LEU:O	1:A:139:LEU:CD2	2.68	0.42
1:A:211:GLY:HA2	1:A:270:TRP:HH2	1.84	0.42
1:A:368:ARG:NH2	1:A:440:GLU:HG3	2.33	0.42
1:A:397:ALA:HB1	1:A:400:LYS:HB2	2.00	0.42
1:A:408:ILE:O	1:A:408:ILE:CG1	2.67	0.42
1:B:7:LEU:O	1:B:8:LEU:C	2.60	0.42
1:B:139:LEU:O	1:B:198:ASN:OD1	2.36	0.42
1:B:149:TRP:HZ2	1:B:192:SER:O	2.01	0.42
1:B:285:MET:C	1:B:287:ILE:N	2.76	0.42
1:A:32:GLN:CD	1:B:138:PRO:HD3	2.44	0.42
1:A:193:HIS:CD2	1:A:214:ILE:CG2	2.93	0.42
1:A:175:TYR:HB3	1:A:569:PHE:CZ	2.53	0.42
1:A:197:ALA:HB3	1:A:210:VAL:HG13	2.01	0.42
1:B:9:ILE:HG13	1:B:65:LEU:HD21	2.02	0.42
1:B:301:TYR:O	1:B:305:LEU:CD2	2.67	0.42
1:B:331:PHE:CE2	1:B:333:ARG:HG2	2.54	0.42
1:B:363:HIS:CE1	1:B:451:ALA:O	2.71	0.42
1:B:414:TYR:C	1:B:415:ILE:HG13	2.45	0.42
1:A:549:GLN:HG3	1:A:553:ARG:HE	1.83	0.42
1:A:79:LEU:HD11	1:A:111:PHE:CZ	2.55	0.42
1:A:311:GLN:HB3	1:A:384:HIS:O	2.19	0.42
1:A:440:GLU:O	1:A:444:ALA:HB2	2.20	0.42
1:B:142:ASP:C	1:B:143:PHE:CD2	2.97	0.42
1:B:543:ASP:O	1:B:547:ALA:HB3	2.19	0.42
1:A:525:ASP:C	1:A:527:ARG:H	2.27	0.42
1:A:540:PHE:CD1	1:A:540:PHE:C	2.98	0.42
1:A:116:LEU:HB3	1:A:120:ARG:NH1	2.34	0.42
1:A:143:PHE:N	1:A:194:LEU:O	2.53	0.42
1:A:221:PRO:O	1:A:241:THR:CG2	2.60	0.42
1:A:221:PRO:HD2	1:A:241:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:VAL:HG22	1:A:418:ARG:HA	2.01	0.42
1:A:465:VAL:HG12	1:A:466:THR:N	2.34	0.42
1:B:143:PHE:CD2	1:B:143:PHE:N	2.88	0.42
1:B:442:GLY:CA	1:B:536:HIS:CD2	2.88	0.42
1:B:448:LEU:O	1:B:453:ILE:N	2.51	0.42
1:B:450:ALA:HB3	1:B:558:GLU:HG2	1.98	0.42
1:A:157:ILE:HG21	1:A:169:LYS:HG3	2.02	0.42
1:A:488:ARG:O	1:A:514:PHE:HD1	1.95	0.42
1:B:475:ASP:C	1:B:477:ASP:H	2.28	0.42
1:A:114:ARG:C	1:A:114:ARG:CD	2.92	0.42
1:A:378:PHE:C	1:A:378:PHE:CD2	2.98	0.42
1:A:489:ASP:CB	1:A:514:PHE:CD1	3.02	0.42
1:B:121:LEU:HD12	1:B:121:LEU:O	2.20	0.42
1:B:226:ILE:HG22	1:B:234:LEU:HD22	2.02	0.42
1:B:459:LEU:O	1:B:463:PHE:HD2	2.03	0.42
1:A:32:GLN:HG3	1:A:202:TYR:OH	2.20	0.41
1:A:200:LEU:HD21	1:A:208:TRP:H	1.85	0.41
1:B:48:LYS:HE2	1:B:362:GLU:CG	2.49	0.41
1:B:403:ASP:O	1:B:404:LEU:HD23	2.19	0.41
1:A:80:LEU:CD2	1:A:119:GLU:O	2.68	0.41
1:A:196:VAL:HG13	1:A:209:LEU:HD23	2.02	0.41
1:A:315:ALA:HB3	1:A:325:VAL:CG1	2.50	0.41
1:A:379:VAL:HG13	1:A:379:VAL:O	2.21	0.41
1:B:95:ARG:HH21	1:B:262:PRO:C	2.21	0.41
1:B:286:ALA:C	1:B:287:ILE:HD12	2.45	0.41
1:A:87:THR:C	1:A:89:LEU:H	2.27	0.41
1:A:248:ILE:O	1:A:249:VAL:C	2.63	0.41
1:A:325:VAL:CG1	2:A:1762:ADP:O4'	2.61	0.41
1:A:390:MET:O	1:A:394:LEU:N	2.35	0.41
1:B:32:GLN:O	1:B:36:GLU:CB	2.68	0.41
1:B:466:THR:HG23	1:B:467:ARG:N	2.34	0.41
1:A:79:LEU:HD11	1:A:111:PHE:CE1	2.55	0.41
1:B:80:LEU:O	1:B:81:ARG:C	2.63	0.41
1:B:354:ARG:HA	1:B:354:ARG:HD3	1.79	0.41
1:B:368:ARG:O	1:B:369:MET:HG2	2.19	0.41
1:B:514:PHE:CD2	1:B:517:GLU:OE2	2.73	0.41
1:A:54:TYR:OH	1:A:102:PHE:HA	2.20	0.41
1:A:69:THR:O	1:A:73:SER:HB2	2.21	0.41
1:A:113:HIS:O	1:A:377:ASN:HB2	2.20	0.41
1:A:157:ILE:CG2	1:A:169:LYS:CD	2.96	0.41
1:B:93:TYR:CB	1:B:96:PHE:HB3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:THR:HG22	1:B:284:TYR:HE2	1.85	0.41
1:B:432:GLN:O	1:B:436:ASP:N	2.34	0.41
1:A:334:VAL:HG23	1:A:416:GLU:O	2.20	0.41
1:A:355:ALA:O	1:A:359:LEU:CB	2.68	0.41
1:A:362:GLU:H	1:A:362:GLU:HG2	1.73	0.41
1:B:68:ILE:CG1	1:B:69:THR:H	2.26	0.41
1:B:78:PHE:CD1	1:B:81:ARG:NH2	2.88	0.41
1:B:340:ASP:OD1	1:B:396:GLU:O	2.37	0.41
1:B:525:ASP:CB	1:B:528:ILE:CD1	2.99	0.41
1:A:222:PHE:CE2	1:A:224:LEU:CD1	3.03	0.41
1:A:279:THR:OG1	1:A:282:GLU:OE1	2.26	0.41
1:A:438:ILE:O	1:A:441:TYR:HB3	2.21	0.41
1:B:253:ALA:C	1:B:367:GLY:HA2	2.46	0.41
1:A:157:ILE:HG21	1:A:169:LYS:CD	2.51	0.41
1:A:166:TRP:O	1:A:167:GLN:OE1	2.38	0.41
1:A:198:ASN:HA	1:A:199:GLU:HA	1.71	0.41
1:A:204:ASN:HB3	1:A:205:LYS:H	1.53	0.41
1:A:509:SER:N	1:A:510:PRO:HD3	2.33	0.41
1:B:58:VAL:HG11	1:B:105:SER:HB2	2.03	0.41
1:B:116:LEU:H	1:B:116:LEU:HG	1.64	0.41
1:B:253:ALA:O	1:B:365:ARG:HB3	2.21	0.41
1:B:541:ARG:HH22	1:B:544:TYR:CB	2.26	0.41
1:A:389:LEU:O	1:A:392:LEU:HD23	2.21	0.41
1:B:57:HIS:O	1:B:61:VAL:HG13	2.21	0.41
1:B:68:ILE:CG1	1:B:69:THR:N	2.79	0.41
1:A:9:ILE:O	1:A:12:THR:HB	2.22	0.40
1:A:107:TYR:OH	1:A:120:ARG:CG	2.69	0.40
1:A:134:THR:HG23	1:A:134:THR:H	1.51	0.40
1:A:143:PHE:O	1:A:194:LEU:O	2.39	0.40
1:A:161:PRO:CB	1:B:138:PRO:HB3	2.49	0.40
1:A:234:LEU:HD13	1:A:234:LEU:H	1.87	0.40
1:A:240:LEU:HD22	1:A:245:GLU:HB3	2.03	0.40
1:B:529:GLY:O	1:B:532:PHE:CB	2.66	0.40
1:B:559:ASP:HB3	1:B:561:TYR:HE2	1.86	0.40
1:A:87:THR:C	1:A:89:LEU:N	2.79	0.40
1:A:250:PHE:CB	1:A:275:LEU:HD21	2.51	0.40
1:B:24:PHE:CE1	1:B:50:ARG:HG2	2.56	0.40
1:B:34:ARG:HD2	1:B:34:ARG:HA	1.93	0.40
1:B:200:LEU:HB3	1:B:208:TRP:O	2.21	0.40
1:B:271:LEU:HB2	1:B:283:LEU:HD11	2.02	0.40
1:B:334:VAL:HG12	1:B:416:GLU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:GLN:C	1:B:551:ARG:H	2.29	0.40
1:A:172:ASP:OD1	1:A:236:ILE:HB	2.21	0.40
1:B:155:ARG:HD3	1:B:155:ARG:HA	1.91	0.40
1:B:203:ARG:NH2	1:B:254:ARG:CG	2.83	0.40
1:B:382:LYS:HD3	1:B:390:MET:HE1	2.02	0.40
1:B:425:TRP:CZ3	1:B:429:VAL:HG21	2.56	0.40
1:B:433:GLN:OE1	1:B:433:GLN:CA	2.68	0.40
1:A:48:LYS:CG	1:A:362:GLU:HB2	2.45	0.40
1:A:229:THR:HB	1:A:233:GLU:CG	2.50	0.40
1:A:305:LEU:CD1	1:A:305:LEU:N	2.72	0.40
1:B:101:SER:HA	1:B:104:ASN:HD22	1.85	0.40
1:B:195:GLN:HB2	1:B:214:ILE:HD11	2.04	0.40
1:A:107:TYR:OH	1:A:120:ARG:HG3	2.21	0.40
1:A:220:LEU:HG	1:A:221:PRO:HD2	1.99	0.40
1:A:226:ILE:HG23	1:A:236:ILE:HG12	2.02	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ASN:ND2	1:B:427:GLU:CD[2_455]	1.48	0.72
1:A:423:ASN:CG	1:B:427:GLU:OE2[2_455]	1.55	0.65
1:A:423:ASN:ND2	1:B:427:GLU:OE1[2_455]	1.74	0.46
1:A:423:ASN:ND2	1:B:427:GLU:OE2[2_455]	1.98	0.22
1:A:423:ASN:CG	1:B:427:GLU:CD[2_455]	2.01	0.19
1:A:423:ASN:OD1	1:B:427:GLU:OE2[2_455]	2.09	0.11
1:A:423:ASN:CB	1:B:427:GLU:OE2[2_455]	2.13	0.07

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	541/578 (94%)	470 (87%)	65 (12%)	6 (1%)	11	39
1	B	529/578 (92%)	457 (86%)	68 (13%)	4 (1%)	16	47
All	All	1070/1156 (93%)	927 (87%)	133 (12%)	10 (1%)	14	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	232	GLY
1	A	366	VAL
1	A	511	GLY
1	B	118	PRO
1	B	566	ARG
1	A	264	PRO
1	A	351	ALA
1	B	90	LEU
1	B	216	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	480/508 (94%)	378 (79%)	102 (21%)	1	5
1	B	472/508 (93%)	355 (75%)	117 (25%)	1	2
All	All	952/1016 (94%)	733 (77%)	219 (23%)	1	4

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	17	PHE
1	A	20	GLN
1	A	25	LEU
1	A	27	VAL
1	A	29	SER

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Mol	Chain	Res	Type
1	A	37	GLN
1	A	43	VAL
1	A	50	ARG
1	A	58	VAL
1	A	61	VAL
1	A	62	VAL
1	A	65	LEU
1	A	70	ASN
1	A	72	GLN
1	A	82	VAL
1	A	84	GLU
1	A	87	THR
1	A	114	ARG
1	A	134	THR
1	A	135	ILE
1	A	151	SER
1	A	154	MET
1	A	158	SER
1	A	163	ARG
1	A	164	LEU
1	A	165	HIS
1	A	167	GLN
1	A	176	ILE
1	A	179	HIS
1	A	181	THR
1	A	189	LEU
1	A	194	LEU
1	A	199	GLU
1	A	209	LEU
1	A	214	ILE
1	A	215	THR
1	A	217	SER
1	A	219	THR
1	A	220	LEU
1	A	222	PHE
1	A	226	ILE
1	A	234	LEU
1	A	238	THR
1	A	239	CYS
1	A	242	THR
1	A	245	GLU
1	A	249	VAL

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Mol	Chain	Res	Type
1	A	254	ARG
1	A	263	LEU
1	A	271	LEU
1	A	273	GLU
1	A	279	THR
1	A	280	THR
1	A	287	ILE
1	A	290	GLN
1	A	305	LEU
1	A	309	ASN
1	A	310	GLU
1	A	322	VAL
1	A	324	LEU
1	A	328	LEU
1	A	331	PHE
1	A	334	VAL
1	A	335	PHE
1	A	336	LYS
1	A	337	VAL
1	A	338	ILE
1	A	339	LYS
1	A	349	SER
1	A	361	LYS
1	A	362	GLU
1	A	365	ARG
1	A	374	GLU
1	A	380	LEU
1	A	383	ARG
1	A	386	SER
1	A	392	LEU
1	A	408	ILE
1	A	409	VAL
1	A	410	ILE
1	A	416	GLU
1	A	438	ILE
1	A	448	LEU
1	A	452	ASN
1	A	458	MET
1	A	461	LYS
1	A	483	THR
1	A	485	VAL
1	A	522	LEU

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Mol	Chain	Res	Type
1	A	525	ASP
1	A	532	PHE
1	A	534	GLU
1	A	541	ARG
1	A	544	TYR
1	A	548	LEU
1	A	549	GLN
1	A	550	ASN
1	A	554	GLU
1	A	557	VAL
1	A	560	VAL
1	A	563	TYR
1	B	3	ARG
1	B	5	LEU
1	B	6	GLU
1	B	7	LEU
1	B	33	GLN
1	B	35	PHE
1	B	44	GLN
1	B	47	MET
1	B	53	LEU
1	B	67	CYS
1	B	72	GLN
1	B	79	LEU
1	B	80	LEU
1	B	81	ARG
1	B	89	LEU
1	B	95	ARG
1	B	96	PHE
1	B	112	ASP
1	B	113	HIS
1	B	116	LEU
1	B	117	THR
1	B	121	LEU
1	B	122	PHE
1	B	124	PHE
1	B	134	THR
1	B	135	ILE
1	B	136	PRO
1	B	141	LYS
1	B	152	LEU
1	B	162	LEU

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Mol	Chain	Res	Type
1	B	171	ARG
1	B	174	HIS
1	B	183	THR
1	B	189	LEU
1	B	212	LYS
1	B	215	THR
1	B	219	THR
1	B	222	PHE
1	B	223	LEU
1	B	228	GLN
1	B	231	ASP
1	B	233	GLU
1	B	241	THR
1	B	243	THR
1	B	245	GLU
1	B	247	SER
1	B	249	VAL
1	B	258	MET
1	B	263	LEU
1	B	275	LEU
1	B	280	THR
1	B	287	ILE
1	B	290	GLN
1	B	291	LYS
1	B	294	LYS
1	B	295	THR
1	B	299	ARG
1	B	305	LEU
1	B	306	GLN
1	B	309	ASN
1	B	321	MET
1	B	324	LEU
1	B	325	VAL
1	B	337	VAL
1	B	341	LYS
1	B	352	HIS
1	B	353	VAL
1	B	354	ARG
1	B	356	CYS
1	B	357	TYR
1	B	359	LEU
1	B	360	VAL

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Mol	Chain	Res	Type
1	B	364	ASP
1	B	368	ARG
1	B	372	THR
1	B	376	GLU
1	B	379	VAL
1	B	383	ARG
1	B	391	GLU
1	B	392	LEU
1	B	393	LEU
1	B	400	LYS
1	B	401	ILE
1	B	402	THR
1	B	404	LEU
1	B	406	GLU
1	B	408	ILE
1	B	409	VAL
1	B	411	ARG
1	B	413	LEU
1	B	417	ARG
1	B	420	VAL
1	B	425	TRP
1	B	426	LEU
1	B	427	GLU
1	B	429	VAL
1	B	430	GLU
1	B	433	GLN
1	B	439	GLU
1	B	447	GLN
1	B	457	ASP
1	B	459	LEU
1	B	466	THR
1	B	472	VAL
1	B	474	TYR
1	B	478	GLU
1	B	479	ILE
1	B	485	VAL
1	B	489	ASP
1	B	516	GLU
1	B	521	TRP
1	B	522	LEU
1	B	531	LEU
1	B	538	ASP

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Mol	Chain	Res	Type
1	B	548	LEU
1	B	564	ARG
1	B	571	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	33	GLN
1	A	45	GLN
1	A	64	GLN
1	A	72	GLN
1	A	85	HIS
1	A	104	ASN
1	A	165	HIS
1	A	204	ASN
1	A	227	HIS
1	A	292	HIS
1	A	309	ASN
1	A	407	GLN
1	A	447	GLN
1	A	536	HIS
1	A	550	ASN
1	B	32	GLN
1	B	45	GLN
1	B	64	GLN
1	B	72	GLN
1	B	85	HIS
1	B	104	ASN
1	B	168	ASN
1	B	179	HIS
1	B	204	ASN
1	B	228	GLN
1	B	290	GLN
1	B	292	HIS
1	B	309	ASN
1	B	363	HIS
1	B	377	ASN
1	B	407	GLN
1	B	412	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 ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	1762	3	28,29,29	1.32	4 (14%)	43,45,45	2.23	10 (23%)
4	AMP	B	1604	-	25,25,25	1.46	3 (12%)	37,38,38	2.16	10 (27%)

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	ADP	A	1762	3	-	5/16/32/32	0/3/3/3
4	AMP	B	1604	-	-	5/10/26/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1604	AMP	C5-C4	4.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1762	ADP	C5-C4	4.04	1.46	1.39
4	B	1604	AMP	C5-C6	3.25	1.50	1.41
2	A	1762	ADP	C5-C6	2.88	1.49	1.41
2	A	1762	ADP	C8-N7	2.68	1.36	1.31
4	B	1604	AMP	C8-N7	2.64	1.36	1.31
2	A	1762	ADP	PA-O3A	2.23	1.61	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1604	AMP	C5-C4-N3	-6.11	118.30	126.72
2	A	1762	ADP	C5-C4-N3	-5.93	118.55	126.72
2	A	1762	ADP	C2'-C1'-N9	-4.93	101.05	113.30
2	A	1762	ADP	N3-C4-N9	4.70	135.16	127.17
2	A	1762	ADP	C2-N3-C4	4.57	122.99	111.83
4	B	1604	AMP	N3-C4-N9	4.46	134.76	127.17
4	B	1604	AMP	C2-N3-C4	4.31	122.35	111.83
2	A	1762	ADP	N3-C2-N1	-4.20	122.23	128.58
4	B	1604	AMP	C4-C5-N7	-4.11	105.88	110.58
4	B	1604	AMP	N3-C2-N1	-3.89	122.69	128.58
2	A	1762	ADP	C4-N9-C8	3.60	109.51	105.74
2	A	1762	ADP	C4-C5-N7	-3.50	106.58	110.58
2	A	1762	ADP	C6-C5-N7	3.38	138.60	132.09
4	B	1604	AMP	C6-C5-N7	3.05	137.96	132.09
2	A	1762	ADP	N9-C8-N7	-3.04	109.62	113.94
4	B	1604	AMP	C5-N7-C8	2.93	108.06	103.45
2	A	1762	ADP	C5-N7-C8	2.88	107.98	103.45
4	B	1604	AMP	C4-N9-C8	2.59	108.45	105.74
4	B	1604	AMP	O4'-C1'-N9	2.48	112.85	108.09
4	B	1604	AMP	N9-C8-N7	-2.31	110.66	113.94

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1762	ADP	C5'-O5'-PA-O2A
2	A	1762	ADP	C5'-O5'-PA-O3A
2	A	1762	ADP	O4'-C4'-C5'-O5'
4	B	1604	AMP	C5'-O5'-P-O2P
4	B	1604	AMP	C5'-O5'-P-O3P
2	A	1762	ADP	C3'-C4'-C5'-O5'
4	B	1604	AMP	O4'-C4'-C5'-O5'

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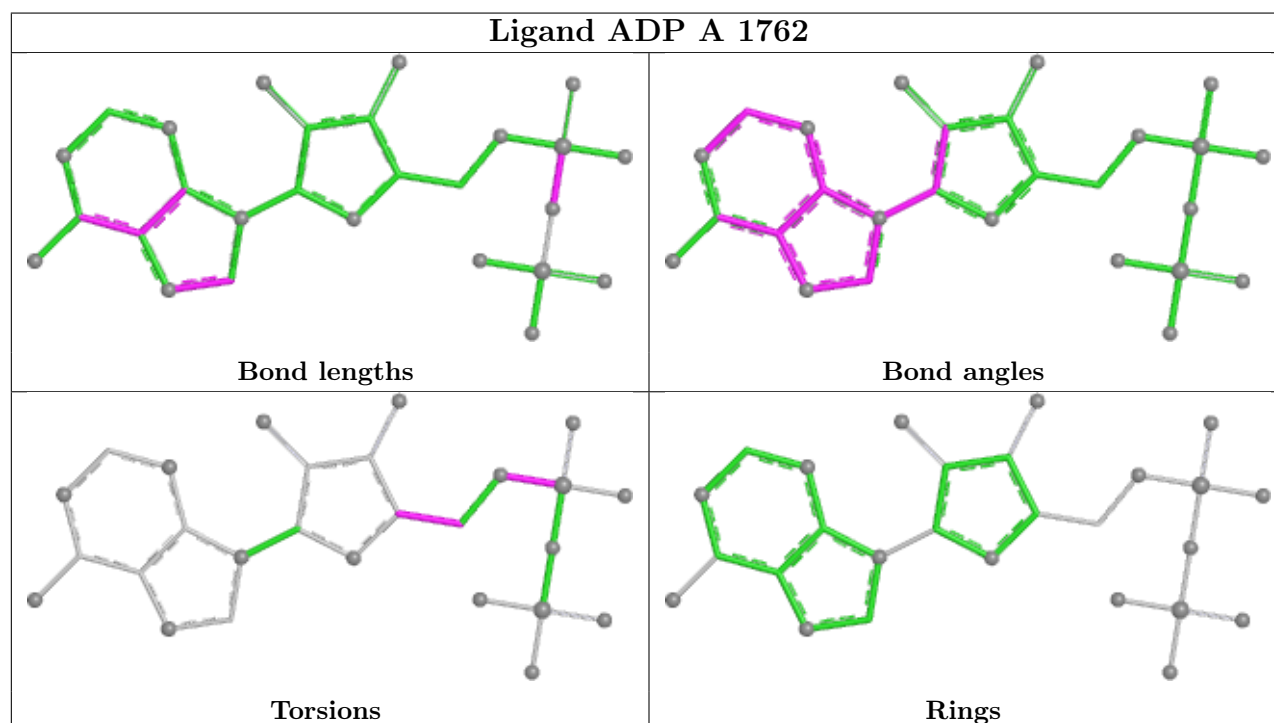
Mol	Chain	Res	Type	Atoms
4	B	1604	AMP	C5'-O5'-P-O1P
4	B	1604	AMP	C3'-C4'-C5'-O5'
2	A	1762	ADP	C5'-O5'-PA-O1A

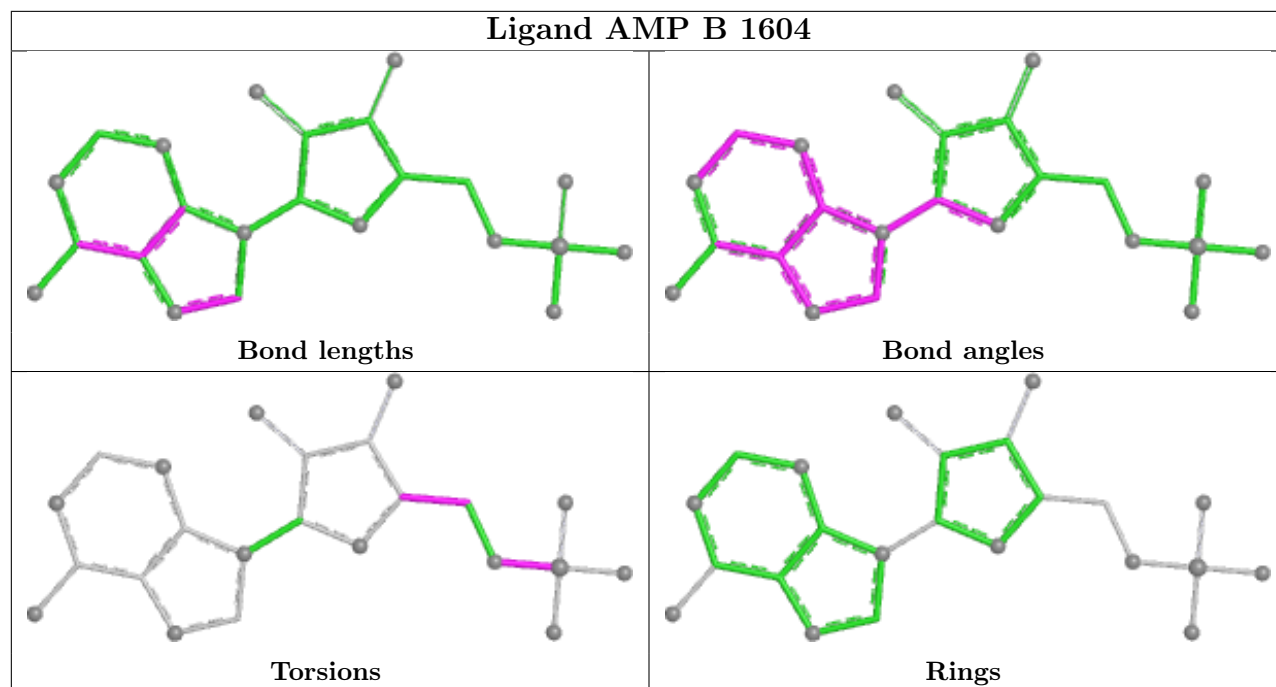
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1762	ADP	5	0
4	B	1604	AMP	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.





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	547/578 (94%)	0.33	15 (2%) 56 35	2, 15, 29, 37	0
1	B	539/578 (93%)	0.44	15 (2%) 55 34	4, 18, 28, 34	0
All	All	1086/1156 (93%)	0.39	30 (2%) 55 34	2, 17, 29, 37	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	THR	4.7
1	B	322	VAL	3.6
1	B	80	LEU	3.4
1	B	456	GLY	3.4
1	A	351	ALA	3.2
1	A	38	ALA	3.1
1	A	158	SER	3.1
1	A	74	THR	2.9
1	A	215	THR	2.9
1	B	38	ALA	2.8
1	A	181	THR	2.8
1	A	145	PRO	2.7
1	A	515	PRO	2.7
1	B	269	GLU	2.6
1	A	486	ASN	2.6
1	A	570	SER	2.4
1	A	386	SER	2.4
1	B	358	GLN	2.4
1	B	25	LEU	2.3
1	B	186	PRO	2.2
1	B	246	ALA	2.2
1	B	234	LEU	2.2
1	B	168	ASN	2.2
1	A	293	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	400	LYS	2.2
1	B	104	ASN	2.2
1	B	310	GLU	2.2
1	A	329	PRO	2.2
1	A	242	THR	2.1
1	B	192	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

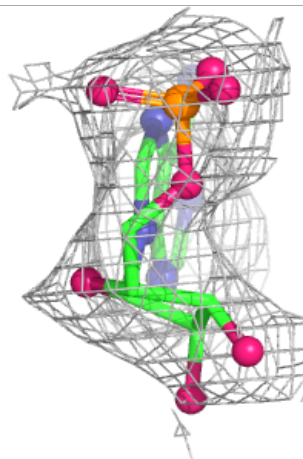
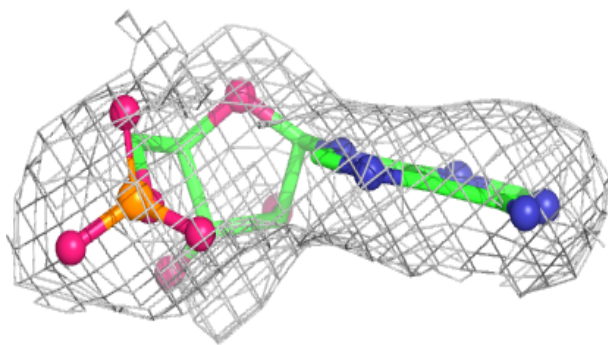
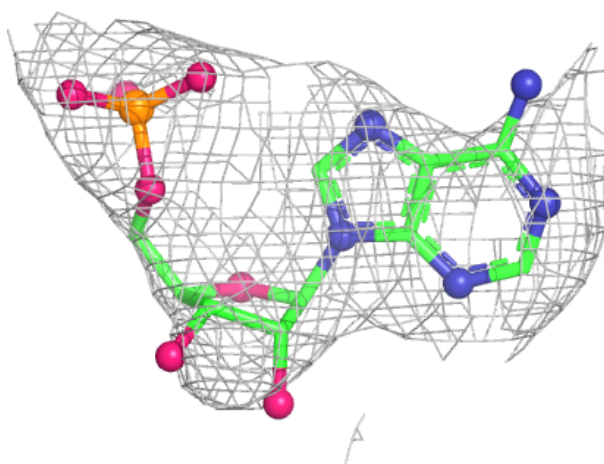
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	AMP	B	1604	23/23	0.89	0.12	23,25,31,34	0
2	ADP	A	1762	27/27	0.95	0.09	6,10,11,12	0
3	MG	A	579	1/1	0.97	0.09	15,15,15,15	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.

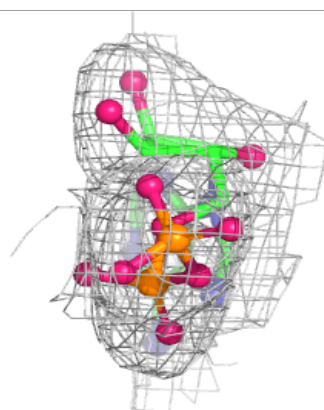
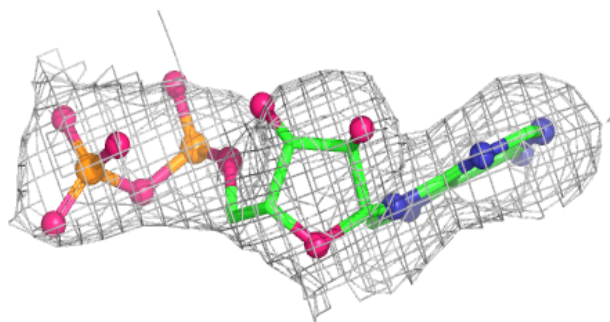
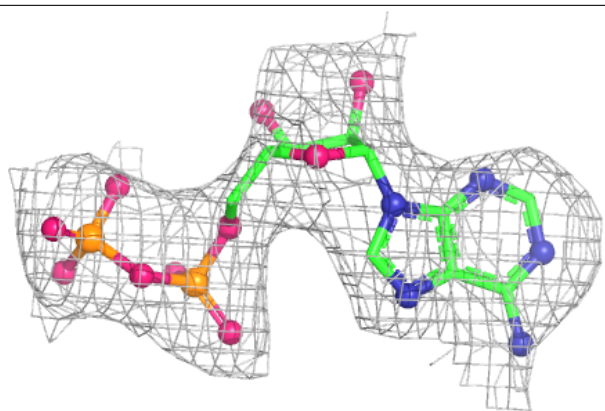
Electron density around AMP B 1604:

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



Electron density around ADP A 1762:

$2mF_o-DF_c$ (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.