



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:28 PM UTC

PDB ID : 4M9S / pdb_00004m9s
Title : crystal structure of CED-4 bound CED-3 fragment
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Deposited on : 2013-08-15
Resolution : 3.21 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

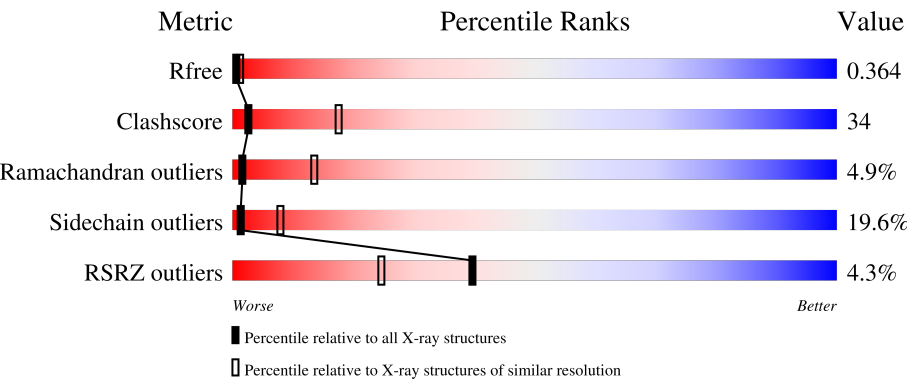
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	549	3% 33%42%16%7%
1	B	549	5% 32%42%16%7%
1	C	549	3% 31%44%17%7%
1	D	549	4% 31%42%17%7%
2	E	8	38%38%25%

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Mol	Chain	Length	Quality of chain
2	F	8	12%38%12%38%
2	G	8	25%12%25%38%
2	H	8	12%38%25%25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16687 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 Cell death protein 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	Se	0	0	0
			4088	2606	685	767	13	17			
1	B	511	Total	C	N	O	S	Se	0	0	0
			4094	2607	688	768	14	17			
1	C	510	Total	C	N	O	S	Se	0	0	0
			4088	2606	685	767	13	17			
1	D	511	Total	C	N	O	S	Se	0	0	0
			4094	2607	688	768	14	17			

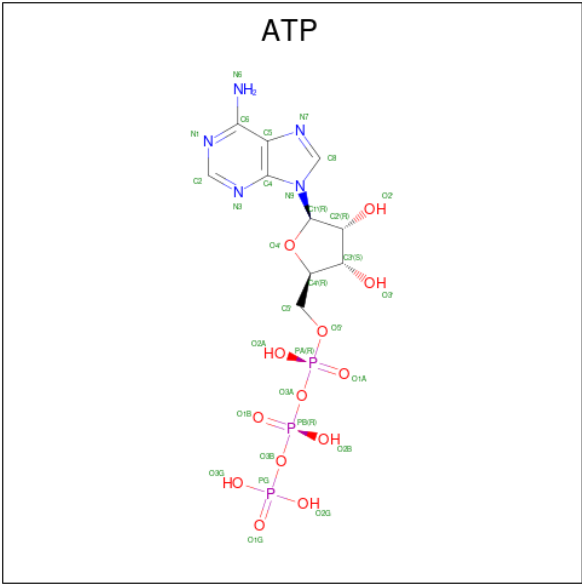
- Molecule 2 is a protein called CED-3 fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	Se	0	0	0
			50	34	7	7	2			
2	F	5	Total	C	N	O	Se	0	0	0
			46	32	6	6	2			
2	G	5	Total	C	N	O	Se	0	0	0
			46	32	6	6	2			
2	H	6	Total	C	N	O	Se	0	0	0
			53	37	7	7	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		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

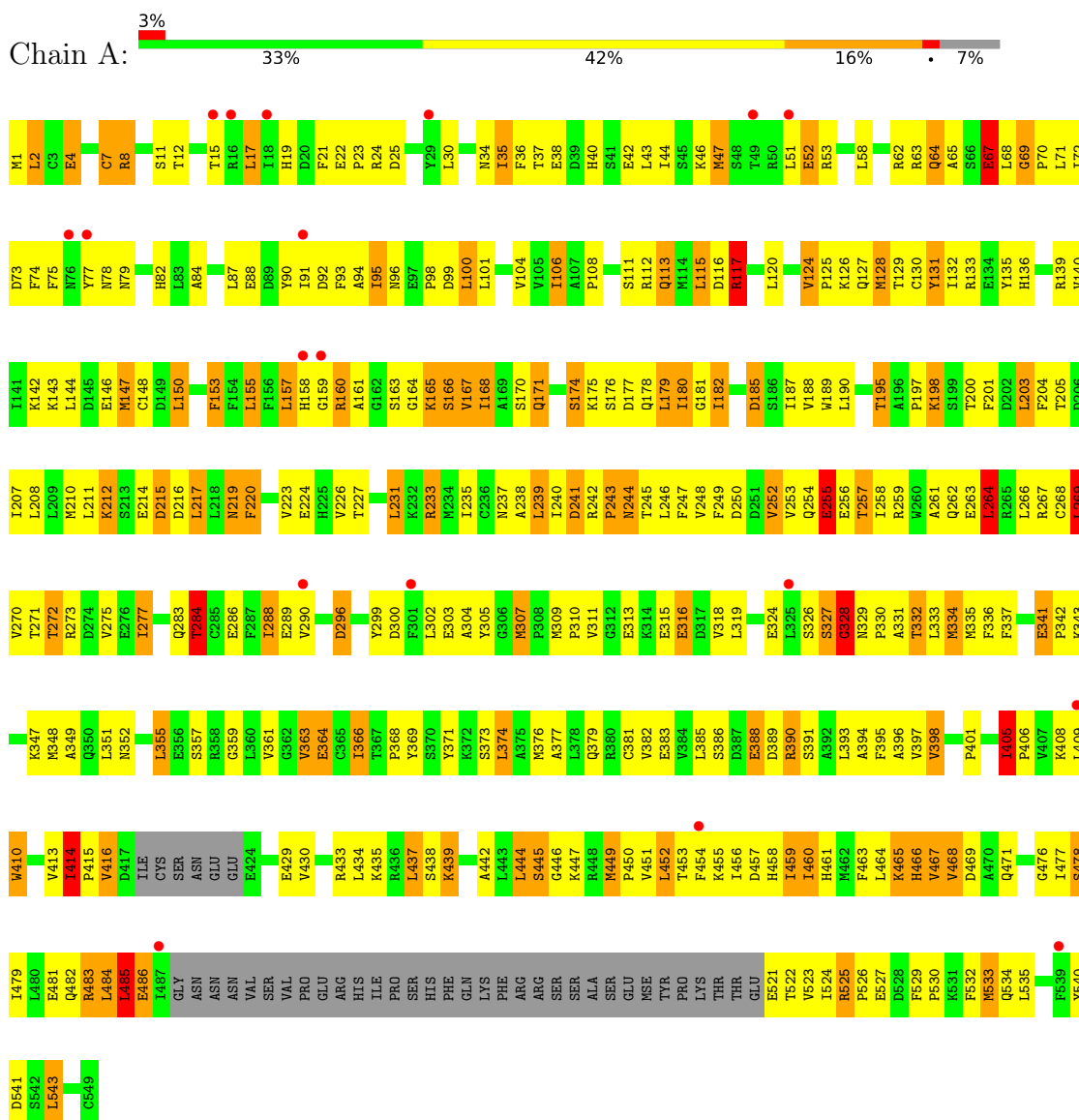


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots

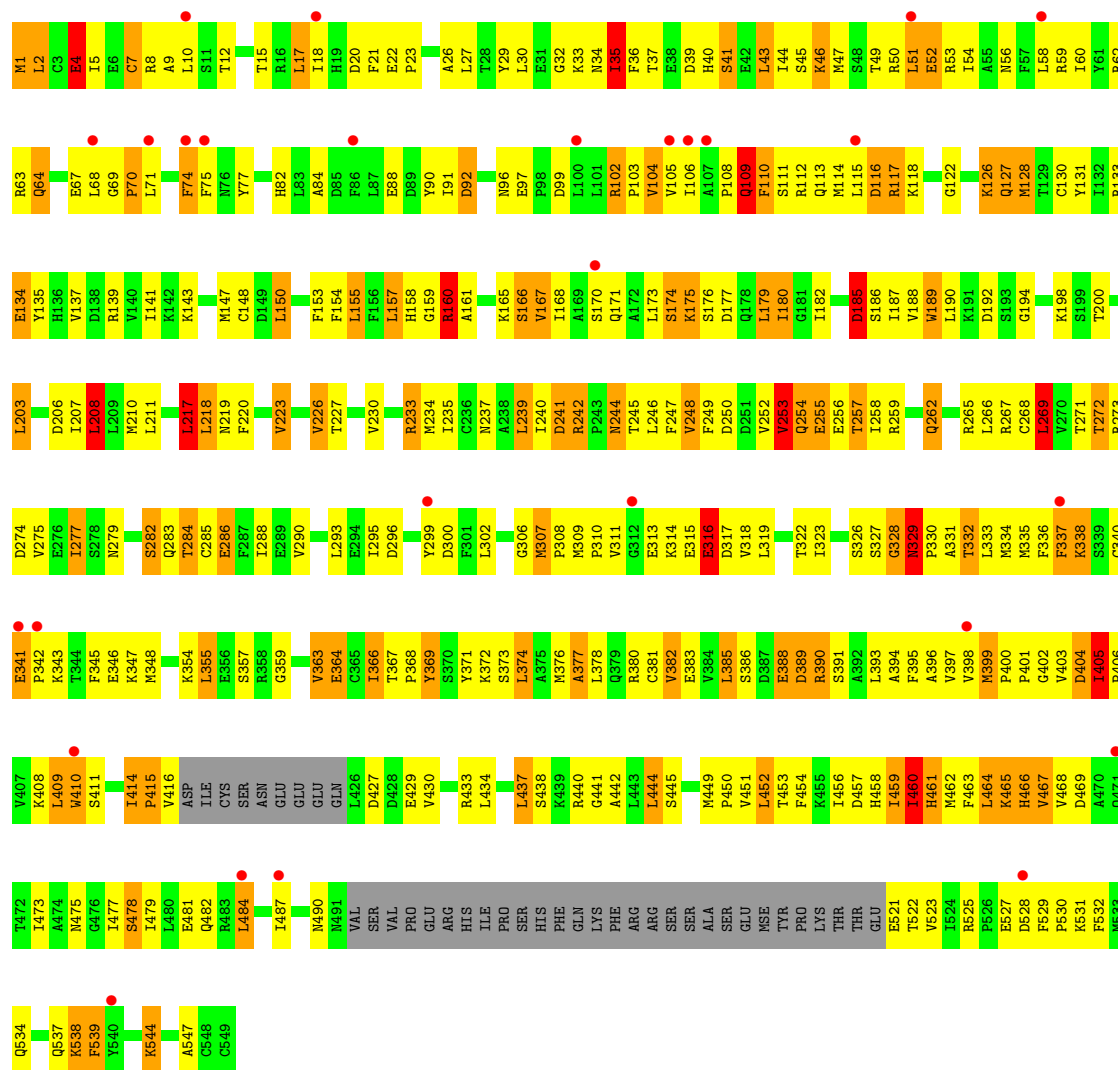
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cell death protein 4



• Molecule 1: Cell death protein 4









- Molecule 2: CED-3 fragment



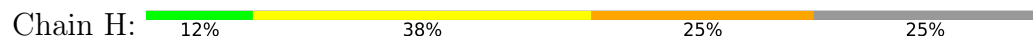
- Molecule 2: CED-3 fragment



- Molecule 2: CED-3 fragment



- Molecule 2: CED-3 fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.81Å 178.81Å 201.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.85 – 3.21 40.85 – 3.21	Depositor EDS
% Data completeness (in resolution range)	55.5 (40.85-3.21) 69.1 (40.85-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.87 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.283 , 0.334 0.314 , 0.364	Depositor DCC
R_{free} test set	1877 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å ²)	73.7	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 88.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	16687	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6626e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, 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	1.07	4/4147 (0.1%)	1.56	72/5577 (1.3%)
1	B	1.05	3/4153 (0.1%)	1.54	59/5585 (1.1%)
1	C	1.01	5/4147 (0.1%)	1.47	63/5577 (1.1%)
1	D	1.03	8/4153 (0.2%)	1.53	56/5585 (1.0%)
2	E	1.19	0/50	1.22	0/62
2	F	1.06	0/46	1.31	0/57
2	G	0.92	0/46	1.38	2/57 (3.5%)
2	H	1.02	0/53	1.29	0/65
All	All	1.04	20/16795 (0.1%)	1.52	252/22565 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	G	0	1
All	All	0	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	ILE	CA-C	-8.59	1.42	1.52
1	C	284	THR	CA-CB	6.89	1.65	1.53
1	D	382	VAL	CA-CB	6.79	1.63	1.54
1	C	387	ASP	CA-C	6.73	1.61	1.52
1	D	270	VAL	CA-CB	6.44	1.62	1.54
1	D	387	ASP	CA-C	5.94	1.60	1.52
1	B	248	VAL	CA-CB	-5.89	1.47	1.54
1	D	367	THR	CA-CB	5.88	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	VAL	CA-CB	-5.67	1.47	1.54
1	D	414	ILE	CA-C	5.66	1.57	1.53
1	C	155	LEU	CA-C	-5.46	1.46	1.52
1	D	101	LEU	CA-C	5.43	1.58	1.53
1	D	180	ILE	CA-C	5.41	1.59	1.52
1	A	439	LYS	CA-C	5.37	1.60	1.52
1	B	390	ARG	CA-C	-5.23	1.45	1.52
1	B	461	HIS	CA-C	5.10	1.58	1.53
1	D	240	ILE	CA-CB	5.05	1.60	1.54
1	C	147	MSE	CA-C	5.05	1.59	1.52
1	C	370	SER	CA-C	5.04	1.59	1.52
1	A	390	ARG	CA-C	-5.03	1.45	1.52

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ARG	CA-C-N	11.71	131.67	119.85
1	A	242	ARG	C-N-CA	11.71	131.67	119.85
1	B	484	LEU	N-CA-C	-11.10	99.15	111.14
1	B	405	ILE	CA-C-N	10.84	132.25	120.11
1	B	405	ILE	C-N-CA	10.84	132.25	120.11
1	D	405	ILE	CA-C-N	10.49	131.86	120.11
1	D	405	ILE	C-N-CA	10.49	131.86	120.11
1	D	242	ARG	CA-C-N	10.07	130.02	119.85
1	D	242	ARG	C-N-CA	10.07	130.02	119.85
1	B	166	SER	N-CA-C	-9.15	101.38	111.36
1	D	463	PHE	N-CA-C	-9.14	100.88	111.03
1	B	150	LEU	N-CA-C	9.10	122.06	110.24
1	C	117	ARG	N-CA-C	9.07	121.99	111.11
1	D	112	ARG	N-CA-C	-9.06	103.06	114.56
1	D	307	MSE	CA-C-N	8.94	129.49	119.83
1	D	307	MSE	C-N-CA	8.94	129.49	119.83
1	C	283	GLN	N-CA-C	8.86	120.37	107.88
1	D	150	LEU	N-CA-C	8.85	121.75	110.24
1	A	540	TYR	N-CA-C	-8.68	103.28	114.04
1	D	484	LEU	N-CA-C	-8.47	101.99	111.14
1	B	399	MSE	CA-C-N	-8.40	111.72	120.38
1	B	399	MSE	C-N-CA	-8.40	111.72	120.38
1	A	405	ILE	CA-C-N	8.33	129.44	120.11
1	A	405	ILE	C-N-CA	8.33	129.44	120.11
1	A	219	ASN	N-CA-C	8.29	122.95	113.01
1	B	206	ASP	N-CA-C	-8.11	103.38	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	414	ILE	N-CA-C	7.98	115.50	108.63
1	C	215	ASP	N-CA-C	-7.96	99.27	110.50
1	D	333	LEU	N-CA-C	-7.85	102.67	111.14
1	A	195	THR	N-CA-C	-7.80	103.60	113.43
1	D	304	ALA	N-CA-C	7.78	120.75	111.33
1	D	240	ILE	N-CA-C	-7.78	103.22	110.53
1	A	269	LEU	N-CA-C	-7.78	96.90	109.96
1	B	45	SER	N-CA-C	7.71	121.94	112.23
1	A	34	ASN	N-CA-C	7.70	119.92	110.91
1	A	328	GLY	CA-C-N	-7.66	113.64	122.52
1	A	328	GLY	C-N-CA	-7.66	113.64	122.52
1	A	439	LYS	N-CA-C	7.56	120.41	111.71
1	A	215	ASP	N-CA-C	-7.54	99.86	110.50
1	D	194	GLY	N-CA-C	7.54	124.42	111.15
1	B	427	ASP	N-CA-C	7.53	121.87	108.24
1	D	268	CYS	N-CA-C	7.48	120.61	108.41
1	D	464	LEU	N-CA-C	7.48	119.44	111.28
1	A	124	VAL	CA-C-N	7.41	127.36	120.03
1	A	124	VAL	C-N-CA	7.41	127.36	120.03
1	A	30	LEU	N-CA-C	7.40	122.44	113.41
1	A	468	VAL	CB-CA-C	-7.36	103.50	111.59
1	A	106	ILE	N-CA-C	7.35	117.86	111.90
1	B	242	ARG	CA-C-N	7.34	127.35	119.78
1	B	242	ARG	C-N-CA	7.34	127.35	119.78
1	B	269	LEU	N-CA-C	-7.34	97.62	109.96
1	C	525	ARG	CA-C-N	7.25	127.21	120.03
1	C	525	ARG	C-N-CA	7.25	127.21	120.03
1	D	377	ALA	N-CA-C	-7.25	102.55	111.40
1	A	243	PRO	CA-C-O	-7.24	112.84	121.67
1	D	400	PRO	CA-C-N	-7.20	112.51	120.14
1	D	400	PRO	C-N-CA	-7.20	112.51	120.14
1	C	414	ILE	CA-C-N	7.08	128.04	120.11
1	C	414	ILE	C-N-CA	7.08	128.04	120.11
1	B	402	GLY	N-CA-C	-7.06	101.06	113.76
1	A	164	GLY	N-CA-C	7.05	125.94	115.64
1	C	30	LEU	N-CA-C	7.02	121.97	113.41
1	A	307	MSE	N-CA-C	7.00	118.98	109.24
1	D	110	PHE	N-CA-C	-6.98	103.68	111.28
1	C	329	ASN	CA-C-N	6.96	128.54	119.84
1	C	329	ASN	C-N-CA	6.96	128.54	119.84
1	C	217	LEU	N-CA-C	-6.91	105.13	113.97
1	A	329	ASN	CA-C-N	6.90	128.46	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	ASN	C-N-CA	6.90	128.46	119.84
1	D	269	LEU	N-CA-C	-6.88	98.40	109.96
1	D	329	ASN	CA-C-N	6.87	128.42	119.84
1	D	329	ASN	C-N-CA	6.87	128.42	119.84
1	D	19	HIS	N-CA-C	6.86	118.41	111.07
1	A	100	LEU	N-CA-C	-6.85	104.65	112.87
1	C	307	MSE	CA-C-N	6.84	127.22	119.83
1	C	307	MSE	C-N-CA	6.84	127.22	119.83
1	D	253	VAL	N-CA-C	6.84	117.44	111.90
1	A	357	SER	N-CA-C	6.79	120.47	112.72
1	D	89	ASP	N-CA-C	-6.78	103.69	112.23
1	A	268	CYS	N-CA-C	6.76	119.92	108.90
1	B	415	PRO	N-CA-C	6.76	121.00	111.33
1	B	389	ASP	N-CA-C	-6.72	104.02	111.82
1	C	106	ILE	N-CA-C	6.71	117.34	111.90
1	B	458	HIS	N-CA-C	6.71	119.94	111.69
1	B	268	CYS	N-CA-C	6.69	119.81	108.90
1	C	212	LYS	N-CA-C	6.68	119.67	110.24
1	A	124	VAL	N-CA-C	-6.66	102.90	108.63
1	B	4	GLU	N-CA-C	6.66	118.62	111.36
1	B	307	MSE	CA-C-N	6.61	126.97	119.83
1	B	307	MSE	C-N-CA	6.61	126.97	119.83
1	A	220	PHE	CA-C-N	6.58	128.03	120.98
1	A	220	PHE	C-N-CA	6.58	128.03	120.98
1	A	71	LEU	N-CA-C	-6.57	106.48	114.75
1	B	333	LEU	N-CA-C	-6.52	104.09	111.07
1	D	523	VAL	N-CA-C	6.51	117.50	108.12
1	A	64	GLN	N-CA-C	6.51	121.50	112.45
1	A	69	GLY	CA-C-N	6.50	127.97	119.84
1	A	69	GLY	C-N-CA	6.50	127.97	119.84
1	B	114	MSE	N-CA-C	6.48	118.01	111.07
1	B	357	SER	N-CA-C	6.48	120.10	112.72
1	D	235	ILE	N-CA-C	-6.42	104.89	110.74
1	D	403	VAL	N-CA-C	6.40	117.52	108.17
1	C	71	LEU	N-CA-C	-6.40	106.69	114.75
1	A	212	LYS	CA-C-N	6.39	131.67	120.87
1	A	212	LYS	C-N-CA	6.39	131.67	120.87
1	A	255	GLU	CA-CB-CG	6.39	126.88	114.10
1	B	538	LYS	CA-CB-CG	-6.38	101.33	114.10
1	C	281	ALA	N-CA-C	6.35	119.06	108.96
1	A	414	ILE	CA-C-N	6.34	127.22	120.11
1	A	414	ILE	C-N-CA	6.34	127.22	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	478	SER	N-CA-C	6.33	117.97	111.14
1	A	478	SER	N-CA-C	6.31	117.96	111.14
1	B	338	LYS	CB-CG-CD	6.30	125.79	111.30
1	C	124	VAL	N-CA-C	-6.30	103.21	108.63
1	C	289	GLU	N-CA-C	6.29	119.50	109.24
1	C	405	ILE	CA-C-N	6.29	127.15	120.11
1	C	405	ILE	C-N-CA	6.29	127.15	120.11
1	D	223	VAL	N-CA-C	6.26	120.90	111.89
1	B	217	LEU	N-CA-C	-6.25	105.97	113.97
1	A	117	ARG	N-CA-C	6.23	118.59	111.11
1	A	129	THR	N-CA-C	6.23	121.47	113.18
1	C	138	ASP	N-CA-C	6.22	117.85	111.14
1	D	16	ARG	N-CA-C	6.19	121.03	111.56
1	C	97	GLU	CA-C-N	6.18	126.64	120.52
1	C	97	GLU	C-N-CA	6.18	126.64	120.52
1	B	185	ASP	N-CA-C	6.18	117.81	111.14
1	A	333	LEU	N-CA-C	-6.17	104.64	111.36
1	C	269	LEU	N-CA-C	-6.16	99.61	109.96
1	C	540	TYR	N-CA-C	-6.15	106.41	114.04
1	D	299	TYR	N-CA-C	-6.13	104.51	111.07
1	C	177	ASP	N-CA-C	-6.11	104.44	113.61
1	A	231	LEU	N-CA-C	-6.10	104.63	111.28
1	D	283	GLN	N-CA-C	6.08	116.46	107.88
1	D	414	ILE	N-CA-C	6.02	113.81	108.63
1	C	309	MSE	N-CA-C	6.01	118.58	110.29
1	B	337	PHE	N-CA-CB	5.99	118.69	110.01
1	C	34	ASN	N-CA-C	5.98	117.91	110.91
1	C	268	CYS	N-CA-C	5.97	118.14	108.41
1	A	541	ASP	N-CA-C	-5.96	104.91	111.82
1	D	534	GLN	N-CA-C	-5.95	105.87	113.01
1	A	284	THR	CA-C-N	-5.94	114.62	122.99
1	A	284	THR	C-N-CA	-5.94	114.62	122.99
1	D	242	ARG	N-CA-C	5.93	120.84	108.39
1	A	463	PHE	N-CA-C	-5.92	104.45	111.03
1	C	64	GLN	N-CA-C	5.92	120.68	112.45
1	A	217	LEU	N-CA-C	-5.88	106.27	113.50
1	A	264	LEU	N-CA-C	-5.87	105.97	113.02
1	A	535	LEU	N-CA-C	-5.85	104.90	111.28
1	D	458	HIS	N-CA-C	5.84	120.57	112.45
1	A	150	LEU	N-CA-C	5.82	117.81	110.24
1	C	299	TYR	N-CA-C	-5.81	104.85	111.07
1	B	253	VAL	N-CA-C	5.80	116.60	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	5	ILE	N-CA-C	5.77	116.42	110.82
1	B	544	LYS	N-CA-C	-5.76	105.08	111.36
1	C	211	LEU	N-CA-C	-5.75	104.38	111.40
1	B	329	ASN	CA-C-N	5.74	127.01	119.84
1	B	329	ASN	C-N-CA	5.74	127.01	119.84
1	B	118	LYS	N-CA-C	5.73	117.61	111.36
1	C	124	VAL	CA-C-N	5.73	125.70	120.03
1	C	124	VAL	C-N-CA	5.73	125.70	120.03
1	A	304	ALA	N-CA-C	5.71	118.24	111.33
1	D	155	LEU	CB-CA-C	-5.71	100.83	110.19
1	A	168	ILE	CB-CA-C	-5.70	104.45	112.14
1	A	166	SER	N-CA-C	-5.68	105.09	111.28
1	B	460	ILE	N-CA-C	-5.67	105.62	113.00
1	D	95	ILE	N-CA-C	5.67	115.75	110.42
1	D	217	LEU	N-CA-C	-5.64	106.75	113.97
1	C	370	SER	CA-C-N	5.64	130.94	122.99
1	C	370	SER	C-N-CA	5.64	130.94	122.99
1	D	343	LYS	N-CA-CB	-5.63	108.47	114.10
1	B	307	MSE	CB-CG-SE	5.62	129.57	112.70
1	B	306	GLY	N-CA-C	5.62	122.59	114.10
1	A	153	PHE	N-CA-C	5.62	117.06	108.52
1	C	404	ASP	N-CA-C	5.62	117.85	109.25
1	D	212	LYS	CA-CB-CG	5.61	125.31	114.10
1	B	316	GLU	N-CA-C	-5.59	105.29	111.71
1	D	459	ILE	CB-CA-C	-5.58	104.61	112.14
1	B	478	SER	N-CA-C	5.58	117.16	111.14
1	C	372	LYS	N-CA-C	5.56	117.34	111.28
1	A	171	GLN	N-CA-C	-5.55	104.86	111.69
1	C	165	LYS	N-CA-C	5.54	117.00	111.07
1	B	456	ILE	CB-CA-C	5.54	119.09	110.83
1	C	80	GLN	N-CA-C	-5.51	104.75	112.25
1	C	463	PHE	N-CA-C	-5.50	104.93	111.03
1	B	282	SER	N-CA-C	5.50	118.31	107.98
1	B	74	PHE	N-CA-C	5.49	118.10	111.40
1	A	147	MSE	N-CA-C	-5.47	106.52	114.12
1	B	7	CYS	N-CA-C	-5.46	105.75	112.90
1	D	129	THR	N-CA-C	5.46	120.44	113.18
1	A	12	THR	N-CA-C	-5.41	105.28	111.07
1	C	212	LYS	CA-CB-CG	5.40	124.91	114.10
1	B	464	LEU	N-CA-C	5.39	117.15	111.28
1	D	206	ASP	N-CA-C	-5.38	106.71	113.28
1	C	164	GLY	CA-C-N	5.38	127.43	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	GLY	C-N-CA	5.38	127.43	120.44
1	A	355	LEU	N-CA-C	5.37	119.00	112.23
1	C	458	HIS	N-CA-C	5.36	118.28	111.69
1	C	212	LYS	CA-C-N	5.35	129.90	120.87
1	C	212	LYS	C-N-CA	5.35	129.90	120.87
1	D	217	LEU	CA-C-N	5.32	127.68	120.44
1	D	217	LEU	C-N-CA	5.32	127.68	120.44
1	C	227	THR	N-CA-C	5.32	117.39	110.43
1	C	153	PHE	N-CA-C	5.30	116.58	108.52
1	B	286	GLU	N-CA-C	-5.28	101.16	109.50
1	C	333	LEU	N-CA-C	-5.26	105.63	111.36
1	A	7	CYS	N-CA-C	-5.25	106.03	112.90
1	A	543	LEU	N-CA-C	5.24	117.07	111.36
1	A	179	LEU	N-CA-C	5.23	117.66	111.33
1	C	389	ASP	N-CA-C	-5.23	105.75	111.82
1	C	430	VAL	CB-CA-C	-5.22	105.29	111.97
1	B	217	LEU	CA-C-N	5.21	127.53	120.44
1	B	217	LEU	C-N-CA	5.21	127.53	120.44
1	C	548	CYS	N-CA-C	-5.21	106.95	113.72
1	B	92	ASP	N-CA-C	-5.19	105.31	111.69
1	B	300	ASP	CA-C-N	5.18	127.75	120.28
1	B	300	ASP	C-N-CA	5.18	127.75	120.28
1	A	288	ILE	CA-C-O	-5.18	115.61	120.22
1	C	486	GLU	N-CA-C	5.17	121.82	110.80
1	B	377	ALA	N-CA-C	-5.16	105.11	111.40
1	B	174	SER	N-CA-C	-5.15	108.02	114.56
1	C	67	GLU	N-CA-C	5.12	115.10	107.88
1	B	385	LEU	N-CA-C	5.12	117.66	110.23
1	D	461	HIS	N-CA-C	-5.12	104.74	111.96
1	A	245	THR	N-CA-C	-5.12	100.83	109.07
1	B	110	PHE	CA-C-N	5.12	128.09	120.31
1	B	110	PHE	C-N-CA	5.12	128.09	120.31
1	D	139	ARG	N-CA-C	-5.12	105.88	111.82
1	D	410	TRP	N-CA-C	-5.12	106.72	113.12
1	A	67	GLU	N-CA-C	5.12	115.09	107.88
1	B	254	GLN	N-CA-C	5.11	117.94	109.46
1	A	300	ASP	CA-C-N	5.10	127.11	120.28
1	A	300	ASP	C-N-CA	5.10	127.11	120.28
2	G	751	ASN	CA-C-N	5.08	131.25	121.54
2	G	751	ASN	C-N-CA	5.08	131.25	121.54
1	C	164	GLY	N-CA-C	5.07	123.05	115.64
1	A	483	ARG	CA-C-N	5.07	131.22	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	ARG	C-N-CA	5.07	131.22	121.54
1	B	427	ASP	CB-CA-C	-5.05	104.37	112.05
1	D	389	ASP	N-CA-C	-5.05	105.96	111.82
1	C	286	GLU	CB-CG-CD	5.05	121.18	112.60
1	D	295	ILE	CB-CA-C	-5.05	104.34	112.16
1	A	414	ILE	N-CA-C	5.04	112.96	108.63
1	D	190	LEU	N-CA-C	5.04	117.27	108.76
1	D	230	VAL	N-CA-C	-5.04	106.24	111.58
1	B	116	ASP	N-CA-CB	5.03	117.24	110.10
1	C	400	PRO	CA-C-N	-5.02	114.82	120.14
1	C	400	PRO	C-N-CA	-5.02	114.82	120.14
1	C	464	LEU	N-CA-C	5.01	116.75	111.28
1	A	165	LYS	N-CA-C	5.01	116.43	111.07
1	A	270	VAL	O-C-N	-5.01	118.46	122.97
1	B	223	VAL	N-CA-C	5.01	119.10	111.89
1	D	154	PHE	N-CA-C	5.00	117.12	109.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	346	GLU	Sidechain
2	G	752	PHE	Peptide

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	4088	0	4107	288	0
1	B	4094	0	4115	280	0
1	C	4088	0	4108	302	1
1	D	4094	0	4115	279	1
2	E	50	0	44	7	0
2	F	46	0	41	6	0
2	G	46	0	41	6	0
2	H	53	0	49	7	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	12	4	0
4	B	31	0	12	5	0
4	C	31	0	12	1	0
4	D	31	0	12	1	0
All	All	16687	0	16668	1135	1

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 34.

All (1135) 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:63:ARG:HE	1:A:240:ILE:HD11	1.24	1.02
1:D:128:MSE:HG3	1:D:167:VAL:HG22	1.48	0.94
1:D:364:GLU:HB2	1:D:373:SER:HB3	1.54	0.89
1:A:484:LEU:HD11	1:A:533:MSE:HG2	1.52	0.89
1:C:63:ARG:HE	1:C:240:ILE:HD11	1.39	0.88
1:A:334:MSE:HE1	1:A:337:PHE:HD2	1.39	0.86
1:D:366:ILE:HD12	1:D:366:ILE:H	1.42	0.85
1:C:190:LEU:HD12	1:C:207:ILE:HG13	1.59	0.84
1:B:366:ILE:HD12	1:B:366:ILE:H	1.43	0.84
1:C:150:LEU:O	1:C:267:ARG:NH1	2.10	0.84
1:D:160:ARG:HG2	1:D:161:ALA:H	1.44	0.83
1:D:397:VAL:HG21	1:D:468:VAL:HG21	1.60	0.82
1:B:75:PHE:HB2	1:B:84:ALA:HB2	1.62	0.82
1:C:138:ASP:OD1	1:C:175:LYS:NZ	2.12	0.82
1:A:128:MSE:HG3	1:A:167:VAL:HG22	1.60	0.82
1:D:160:ARG:NH1	1:D:442:ALA:O	2.12	0.81
1:B:20:ASP:OD2	1:B:82:HIS:NE2	2.13	0.81
1:B:478:SER:O	1:B:482:GLN:HG2	1.80	0.81
1:A:190:LEU:HD12	1:A:207:ILE:HG13	1.62	0.81
1:D:8:ARG:NH1	1:D:90:TYR:OH	2.14	0.81
1:B:165:LYS:HG2	1:B:290:VAL:HG21	1.61	0.81
1:D:190:LEU:HD11	1:D:207:ILE:HG13	1.63	0.81
1:C:484:LEU:HD11	1:C:533:MSE:HG2	1.62	0.80
1:B:128:MSE:HG3	1:B:167:VAL:HG22	1.62	0.80
1:B:102:ARG:HG3	1:B:103:PRO:HD2	1.64	0.79
1:C:47:MSE:HB2	1:C:53:ARG:HG3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PHE:HB2	1:A:84:ALA:HB2	1.64	0.79
1:D:42:GLU:O	1:D:46:LYS:NZ	2.15	0.79
1:D:462:MSE:H	1:D:462:MSE:SE	2.16	0.78
1:C:90:TYR:HE2	1:C:106:ILE:HD11	1.48	0.78
1:C:155:LEU:HB3	1:C:269:LEU:HD23	1.65	0.78
1:B:147:MSE:HE1	1:B:286:GLU:HG2	1.63	0.78
1:C:465:LYS:HD3	1:C:466:HIS:CE1	2.19	0.78
1:C:309:MSE:HG3	1:C:310:PRO:HD2	1.65	0.77
1:C:327:SER:HB2	1:C:459:ILE:HG13	1.66	0.77
1:A:190:LEU:CD1	1:A:207:ILE:HG13	2.16	0.76
1:B:397:VAL:HG21	1:B:468:VAL:HG21	1.66	0.76
1:C:366:ILE:HD12	1:C:366:ILE:H	1.51	0.76
1:A:90:TYR:HE2	1:A:106:ILE:HD11	1.48	0.75
1:C:355:LEU:HD21	1:C:363:VAL:HB	1.69	0.75
1:A:410:TRP:HD1	1:A:414:ILE:HD13	1.52	0.75
1:A:72:ILE:HG21	1:A:88:GLU:HG3	1.67	0.75
1:A:452:LEU:HD23	1:A:452:LEU:H	1.49	0.75
1:D:148:CYS:SG	1:D:183:ASN:ND2	2.58	0.75
1:C:75:PHE:HB2	1:C:84:ALA:HB2	1.68	0.74
2:G:750:PHE:O	2:G:752:PHE:N	2.20	0.74
1:B:92:ASP:OD1	1:B:96:ASN:ND2	2.20	0.73
1:B:449:MSE:HE3	1:B:450:PRO:HA	1.68	0.73
2:F:751:ASN:ND2	2:F:751:ASN:O	2.21	0.73
1:C:41:SER:O	1:C:45:SER:OG	2.07	0.73
1:C:465:LYS:HD3	1:C:466:HIS:HE1	1.54	0.72
1:A:8:ARG:HG2	1:A:8:ARG:HH11	1.55	0.72
1:D:250:ASP:HA	1:D:271:THR:OG1	1.89	0.72
1:A:67:GLU:HG2	1:A:69:GLY:H	1.55	0.72
1:A:334:MSE:HE3	1:A:334:MSE:HA	1.71	0.72
1:A:414:ILE:HG21	1:A:430:VAL:HG13	1.72	0.72
1:B:332:THR:O	1:B:336:PHE:HB2	1.90	0.72
1:B:335:MSE:HE3	1:B:364:GLU:HA	1.71	0.72
1:C:447:LYS:HE2	1:C:450:PRO:HD2	1.71	0.72
1:A:309:MSE:HG3	1:A:310:PRO:HD2	1.71	0.72
1:D:487:ILE:O	1:D:531:LYS:NZ	2.23	0.72
1:C:8:ARG:HG2	1:C:8:ARG:HH11	1.55	0.72
1:D:406:PRO:HA	1:D:453:THR:HG22	1.72	0.72
1:A:128:MSE:HG3	1:A:167:VAL:CG2	2.20	0.71
1:C:128:MSE:HE3	1:D:282:SER:HB2	1.73	0.71
1:C:443:LEU:O	1:C:460:ILE:HG12	1.90	0.71
1:D:40:HIS:HA	1:D:43:LEU:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:O	1:A:267:ARG:NH1	2.24	0.71
1:A:393:LEU:HB2	1:A:437:LEU:HD11	1.73	0.71
1:C:397:VAL:HG22	1:C:464:LEU:HB3	1.71	0.71
1:B:190:LEU:HD12	1:B:207:ILE:HG13	1.71	0.71
1:C:532:PHE:HB2	1:C:534:GLN:HG2	1.73	0.71
1:A:532:PHE:HB2	1:A:534:GLN:HG2	1.72	0.71
1:D:190:LEU:CD1	1:D:207:ILE:HG13	2.20	0.71
1:C:128:MSE:HG3	1:C:167:VAL:HG22	1.72	0.71
1:C:58:LEU:O	1:C:62:ARG:HG3	1.90	0.70
2:E:750:PHE:O	2:E:752:PHE:N	2.24	0.70
1:A:187:ILE:HD13	1:A:246:LEU:HB3	1.73	0.70
1:D:230:VAL:HG12	1:D:234:MSE:HE2	1.74	0.70
1:D:292:SER:HB3	1:D:328:GLY:HA3	1.74	0.70
1:B:1:MSE:HA	1:B:62:ARG:O	1.92	0.70
1:B:335:MSE:HE2	1:B:363:VAL:HG13	1.74	0.70
1:A:449:MSE:HE2	1:A:450:PRO:HA	1.74	0.70
1:A:157:LEU:HD11	1:A:168:ILE:HG22	1.74	0.70
1:A:401:PRO:HB2	1:A:458:HIS:ND1	2.07	0.70
1:B:405:ILE:HG12	1:B:410:TRP:CZ3	2.26	0.69
1:A:47:MSE:HB2	1:A:53:ARG:HG3	1.74	0.69
1:A:406:PRO:HA	1:A:453:THR:HG22	1.74	0.69
1:B:403:VAL:HG12	1:B:405:ILE:HG22	1.74	0.69
1:C:211:LEU:HD13	1:C:239:LEU:HD23	1.75	0.69
1:A:72:ILE:HD11	1:A:87:LEU:HB2	1.74	0.69
1:A:447:LYS:HE2	1:A:450:PRO:HD2	1.74	0.69
1:C:247:PHE:CE2	1:C:266:LEU:HD13	2.28	0.68
1:C:96:ASN:O	1:C:98:PRO:HD3	1.93	0.68
1:B:160:ARG:HG2	1:B:161:ALA:H	1.58	0.68
1:B:102:ARG:HG3	1:B:103:PRO:CD	2.24	0.68
1:C:133:ARG:O	1:C:137:VAL:HG23	1.94	0.68
1:D:128:MSE:HG3	1:D:167:VAL:CG2	2.22	0.68
1:A:160:ARG:HG2	1:A:161:ALA:H	1.58	0.68
1:C:35:ILE:HG12	1:C:65:ALA:HA	1.74	0.68
1:A:247:PHE:CE2	1:A:266:LEU:HD13	2.30	0.67
1:A:334:MSE:HE1	1:A:337:PHE:CD2	2.28	0.67
1:A:389:ASP:HB3	1:A:437:LEU:HD21	1.76	0.67
1:D:155:LEU:HB3	1:D:269:LEU:HD23	1.74	0.67
1:A:386:SER:OG	1:A:388:GLU:OE1	2.12	0.67
1:D:214:GLU:N	1:D:214:GLU:OE1	2.26	0.67
1:D:403:VAL:HG12	1:D:405:ILE:HG22	1.76	0.67
1:B:529:PHE:HB3	1:B:532:PHE:CZ	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HG12	1:A:65:ALA:HA	1.76	0.67
1:B:438:SER:O	1:B:442:ALA:HA	1.95	0.67
1:B:247:PHE:CE2	1:B:266:LEU:HD13	2.29	0.67
1:B:157:LEU:HD11	1:B:168:ILE:HG21	1.75	0.67
1:B:388:GLU:HB3	1:B:433:ARG:HH21	1.59	0.67
1:D:283:GLN:C	1:D:285:CYS:H	2.03	0.67
1:A:96:ASN:O	1:A:98:PRO:HD3	1.94	0.67
1:B:4:GLU:O	1:B:8:ARG:HB2	1.95	0.66
1:D:262:GLN:HE21	1:D:283:GLN:HG3	1.60	0.66
1:A:397:VAL:HG22	1:A:464:LEU:HB3	1.77	0.66
1:C:128:MSE:SE	1:C:167:VAL:HG21	2.45	0.66
1:C:247:PHE:CD2	1:C:266:LEU:HD13	2.31	0.65
1:B:302:LEU:HD13	1:B:319:LEU:HD11	1.76	0.65
1:C:90:TYR:CE2	1:C:106:ILE:HD11	2.32	0.65
1:C:249:PHE:HE2	1:C:261:ALA:HB2	1.61	0.65
1:B:23:PRO:HG2	1:B:53:ARG:C	2.21	0.65
1:D:452:LEU:HD23	1:D:452:LEU:H	1.61	0.65
1:A:438:SER:O	1:A:442:ALA:HA	1.97	0.65
1:A:366:ILE:HD12	1:A:366:ILE:H	1.62	0.65
1:B:464:LEU:O	1:B:468:VAL:HG22	1.97	0.65
1:D:327:SER:HB2	1:D:459:ILE:HG13	1.77	0.65
1:A:165:LYS:N	4:A:602:ATP:O2B	2.30	0.64
1:A:465:LYS:HD3	1:A:466:HIS:CE1	2.32	0.64
1:C:44:ILE:O	1:C:53:ARG:HG2	1.98	0.64
1:C:67:GLU:HG2	1:C:69:GLY:H	1.63	0.64
1:B:406:PRO:HA	1:B:453:THR:HG22	1.80	0.64
1:C:326:SER:O	1:C:328:GLY:N	2.30	0.64
1:A:47:MSE:HE2	1:A:52:GLU:HG2	1.80	0.64
1:C:126:LYS:NZ	1:D:283:GLN:HG2	2.13	0.64
1:D:447:LYS:NZ	1:D:449:MSE:O	2.25	0.64
1:D:2:LEU:HD11	1:D:62:ARG:HE	1.63	0.64
1:C:197:PRO:HD2	1:C:198:LYS:HE2	1.80	0.63
1:A:117:ARG:HH21	1:A:120:LEU:HD23	1.62	0.63
1:B:410:TRP:HD1	1:B:414:ILE:HD13	1.64	0.63
1:C:160:ARG:NH1	1:C:442:ALA:O	2.32	0.63
1:C:341:GLU:HB2	1:C:342:PRO:HD3	1.80	0.63
1:C:434:LEU:HD22	1:C:444:LEU:CD2	2.29	0.63
1:C:214:GLU:OE1	1:C:214:GLU:N	2.27	0.63
1:C:527:GLU:HA	1:C:530:PRO:HG3	1.80	0.63
1:D:30:LEU:HD21	1:D:70:PRO:HB2	1.81	0.63
1:C:349:ALA:HA	1:C:352:ASN:HD22	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LYS:O	1:B:147:MSE:HE3	1.99	0.63
1:B:128:MSE:HG3	1:B:167:VAL:CG2	2.28	0.63
1:A:255:GLU:HA	1:A:277:ILE:HG22	1.80	0.62
1:B:334:MSE:HE2	1:B:338:LYS:CD	2.29	0.62
1:A:335:MSE:HE2	1:A:363:VAL:HG13	1.81	0.62
1:B:135:TYR:O	1:B:139:ARG:HG3	2.00	0.62
1:C:132:ILE:HG23	1:C:137:VAL:HG21	1.80	0.62
1:D:341:GLU:HB2	1:D:342:PRO:HD3	1.80	0.62
1:B:371:TYR:CD2	1:B:377:ALA:HB2	2.34	0.62
1:D:374:LEU:HD13	1:D:374:LEU:O	1.99	0.62
1:A:178:GLN:O	1:A:182:ILE:HB	1.98	0.62
1:D:462:MSE:SE	1:D:462:MSE:N	2.83	0.62
1:A:233:ARG:HG3	1:A:233:ARG:HH11	1.65	0.62
1:B:50:ARG:HA	1:B:53:ARG:HE	1.64	0.62
1:A:8:ARG:NH2	1:A:181:GLY:O	2.29	0.62
1:A:216:ASP:HA	1:A:219:ASN:HB2	1.81	0.62
1:B:309:MSE:HG3	1:B:310:PRO:HD2	1.81	0.62
1:C:434:LEU:HD22	1:C:444:LEU:HD21	1.81	0.62
1:C:469:ASP:HB2	2:G:749:MSE:HA	1.81	0.62
1:D:371:TYR:CD2	1:D:377:ALA:HB2	2.34	0.62
1:B:527:GLU:N	1:B:527:GLU:OE1	2.33	0.62
1:D:178:GLN:HA	1:D:182:ILE:HB	1.82	0.62
1:D:309:MSE:HG3	1:D:310:PRO:HD2	1.81	0.62
1:C:464:LEU:O	1:C:468:VAL:HG22	2.00	0.61
1:D:342:PRO:O	1:D:343:LYS:HB3	2.00	0.61
1:A:252:VAL:HG21	1:A:257:THR:HG21	1.82	0.61
1:C:63:ARG:HE	1:C:240:ILE:CD1	2.12	0.61
1:C:147:MSE:O	1:C:150:LEU:HB2	2.00	0.61
1:C:211:LEU:CD1	1:C:239:LEU:HD23	2.31	0.61
1:D:24:ARG:HG3	1:D:27:LEU:HD12	1.81	0.61
1:A:477:ILE:HD11	1:A:543:LEU:HB3	1.83	0.61
1:C:143:LYS:O	1:C:147:MSE:HG3	2.00	0.61
1:C:410:TRP:HD1	1:C:414:ILE:HD13	1.64	0.61
1:A:401:PRO:HB2	1:A:458:HIS:CE1	2.36	0.61
1:A:397:VAL:O	1:A:461:HIS:NE2	2.29	0.61
1:C:17:LEU:HD23	1:C:21:PHE:CD2	2.35	0.61
1:A:481:GLU:HA	1:A:484:LEU:HD22	1.82	0.61
1:A:247:PHE:HE2	1:A:266:LEU:HD22	1.65	0.61
1:C:142:LYS:O	1:C:146:GLU:HG3	2.00	0.61
1:A:435:LYS:NZ	1:A:446:GLY:HA3	2.16	0.61
1:A:116:ASP:OD1	1:A:116:ASP:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:HB2	1:A:373:SER:HB3	1.83	0.60
1:A:430:VAL:O	1:A:434:LEU:HG	2.02	0.60
1:C:136:HIS:O	1:C:140:VAL:HG23	2.01	0.60
1:C:178:GLN:HA	1:C:182:ILE:HB	1.82	0.60
1:B:430:VAL:O	1:B:434:LEU:HG	2.02	0.60
1:C:397:VAL:HG21	1:C:468:VAL:HG21	1.82	0.60
1:B:364:GLU:HB2	1:B:373:SER:HB3	1.84	0.60
1:C:250:ASP:HA	1:C:271:THR:OG1	2.02	0.60
1:D:430:VAL:O	1:D:434:LEU:HG	2.02	0.60
1:A:211:LEU:HD11	1:A:239:LEU:HD23	1.83	0.60
1:A:214:GLU:HG3	1:B:237:ASN:CG	2.27	0.59
1:D:360:LEU:HD11	1:D:459:ILE:HG22	1.84	0.59
1:C:477:ILE:HG21	1:C:544:LYS:HE3	1.84	0.59
1:B:8:ARG:HH11	1:B:8:ARG:HG2	1.65	0.59
1:B:385:LEU:O	1:B:390:ARG:NH2	2.35	0.59
1:D:141:ILE:HD12	1:D:175:LYS:HE3	1.85	0.59
1:D:464:LEU:O	1:D:468:VAL:HG22	2.03	0.59
1:C:414:ILE:HG21	1:C:430:VAL:HG13	1.83	0.59
1:C:233:ARG:HH11	1:C:233:ARG:HG3	1.67	0.59
1:B:147:MSE:CE	1:B:286:GLU:HG2	2.33	0.59
1:C:40:HIS:O	1:C:44:ILE:HG13	2.02	0.59
1:A:163:SER:C	1:A:330:PRO:HG2	2.28	0.59
1:D:491:ASN:N	1:D:491:ASN:OD1	2.36	0.59
1:A:143:LYS:O	1:A:147:MSE:HG3	2.03	0.58
1:B:165:LYS:N	4:B:602:ATP:O2B	2.36	0.58
1:D:459:ILE:HD12	1:D:460:ILE:H	1.68	0.58
1:A:36:PHE:CD2	1:A:40:HIS:HB3	2.38	0.58
1:A:385:LEU:HD22	1:A:389:ASP:CB	2.33	0.58
1:B:4:GLU:HG3	1:B:5:ILE:N	2.17	0.58
1:A:157:LEU:HD11	1:A:168:ILE:CG2	2.32	0.58
1:A:247:PHE:HB2	1:A:267:ARG:O	2.03	0.58
1:A:341:GLU:HB2	1:A:342:PRO:HD3	1.85	0.58
1:B:190:LEU:CD1	1:B:207:ILE:HG13	2.33	0.58
1:D:189:TRP:CE3	1:D:248:VAL:HG11	2.38	0.58
1:A:40:HIS:O	1:A:44:ILE:HG13	2.03	0.58
1:A:257:THR:HG22	1:A:258:ILE:HD12	1.85	0.58
1:A:305:TYR:OH	4:A:602:ATP:H2	1.87	0.58
1:D:319:LEU:HD12	1:D:345:PHE:CE1	2.37	0.58
1:D:477:ILE:HD13	1:D:544:LYS:HG3	1.85	0.58
1:D:310:PRO:HA	1:D:345:PHE:HE2	1.67	0.58
1:B:315:GLU:HA	1:B:318:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LEU:O	1:B:374:LEU:HD13	2.04	0.58
1:C:529:PHE:HB3	1:C:532:PHE:CZ	2.39	0.58
1:B:47:MSE:HB2	1:B:53:ARG:HG3	1.85	0.58
1:A:262:GLN:O	1:A:262:GLN:HG2	2.02	0.58
1:A:176:SER:OG	1:A:178:GLN:HB2	2.04	0.58
1:A:327:SER:HB2	1:A:459:ILE:HG13	1.85	0.58
1:A:332:THR:HG23	1:A:374:LEU:HB2	1.85	0.58
1:B:395:PHE:HD2	1:B:415:PRO:HD3	1.69	0.58
1:C:216:ASP:H	1:C:218:LEU:HD23	1.68	0.58
1:A:410:TRP:CD1	1:A:414:ILE:HD13	2.36	0.58
1:A:529:PHE:HB3	1:A:532:PHE:CZ	2.38	0.58
1:B:30:LEU:HB3	1:B:36:PHE:CD1	2.39	0.58
1:B:35:ILE:HD12	1:B:70:PRO:HG2	1.86	0.58
1:B:299:TYR:HA	1:B:302:LEU:HD12	1.86	0.58
1:B:341:GLU:HB2	1:B:342:PRO:HD3	1.86	0.58
1:B:399:MSE:HE1	1:B:409:LEU:O	2.03	0.58
1:C:301:PHE:CE1	1:C:305:TYR:HE2	2.21	0.58
1:A:128:MSE:HE3	1:B:282:SER:HB2	1.84	0.57
1:A:385:LEU:HD22	1:A:389:ASP:HB3	1.84	0.57
1:B:185:ASP:N	1:B:244:ASN:O	2.31	0.57
1:C:126:LYS:HZ3	1:D:283:GLN:HG2	1.68	0.57
1:B:248:VAL:HG22	1:B:269:LEU:HB3	1.86	0.57
1:C:139:ARG:NH2	1:C:143:LYS:HE3	2.19	0.57
1:C:395:PHE:CD2	1:C:415:PRO:HD3	2.40	0.57
1:A:143:LYS:HB3	1:A:147:MSE:HE2	1.85	0.57
1:A:189:TRP:CD2	1:A:248:VAL:HG11	2.39	0.57
1:B:158:HIS:CD2	1:B:275:VAL:HG13	2.38	0.57
1:C:23:PRO:HG2	1:C:53:ARG:HB3	1.86	0.57
1:C:26:ALA:HA	1:C:74:PHE:CE1	2.39	0.57
1:D:235:ILE:O	1:D:239:LEU:HB2	2.04	0.57
1:B:111:SER:O	1:B:115:LEU:HB3	2.04	0.57
1:B:235:ILE:O	1:B:239:LEU:HB2	2.05	0.57
1:C:93:PHE:CE2	1:C:100:LEU:HD23	2.40	0.57
1:A:67:GLU:HG2	1:A:69:GLY:N	2.18	0.57
1:B:469:ASP:HB2	2:F:749:MSE:HA	1.87	0.57
1:B:157:LEU:HD11	1:B:168:ILE:CG2	2.35	0.57
1:B:314:LYS:HA	1:B:317:ASP:HB2	1.87	0.57
1:A:393:LEU:O	1:A:393:LEU:HD23	2.04	0.56
1:C:160:ARG:HG2	1:C:161:ALA:H	1.68	0.56
1:B:382:VAL:HA	1:B:385:LEU:HD12	1.86	0.56
1:C:327:SER:HB2	1:C:459:ILE:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:LEU:HD13	1:D:378:LEU:HG	1.86	0.56
1:D:401:PRO:HB2	1:D:458:HIS:CE1	2.41	0.56
1:C:177:ASP:O	1:C:182:ILE:HD13	2.05	0.56
1:D:21:PHE:O	1:D:50:ARG:NE	2.38	0.56
1:D:200:THR:HG21	1:D:256:GLU:HB3	1.87	0.56
1:D:436:ARG:O	1:D:440:ARG:HG3	2.06	0.56
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.71	0.56
1:B:293:LEU:HG	1:B:330:PRO:HD3	1.87	0.56
1:C:216:ASP:HA	1:C:219:ASN:HB2	1.87	0.56
1:D:334:MSE:CE	1:D:337:PHE:HB3	2.36	0.56
1:A:23:PRO:HG2	1:A:53:ARG:HB3	1.87	0.56
1:B:133:ARG:O	1:B:137:VAL:HG23	2.06	0.56
1:D:7:CYS:O	1:D:11:SER:OG	2.11	0.56
1:D:157:LEU:HD11	1:D:168:ILE:HG22	1.87	0.56
1:A:158:HIS:CE1	1:A:289:GLU:HB2	2.39	0.55
1:B:257:THR:HG22	1:B:258:ILE:N	2.21	0.55
1:B:473:ILE:HG22	1:B:547:ALA:HB2	1.87	0.55
1:C:37:THR:O	1:C:40:HIS:HB2	2.05	0.55
1:C:247:PHE:HB2	1:C:267:ARG:O	2.07	0.55
1:C:274:ASP:O	1:C:277:ILE:HG12	2.06	0.55
1:D:388:GLU:O	1:D:391:SER:OG	2.13	0.55
1:C:200:THR:HG21	1:C:256:GLU:HB3	1.88	0.55
1:D:214:GLU:N	1:D:214:GLU:CD	2.64	0.55
1:A:58:LEU:O	1:A:62:ARG:HG3	2.05	0.55
1:A:147:MSE:O	1:A:150:LEU:HB2	2.05	0.55
1:C:343:LYS:O	1:C:343:LYS:HG2	2.05	0.55
1:C:467:VAL:O	2:G:751:ASN:HB2	2.06	0.55
1:D:187:ILE:HD13	1:D:246:LEU:HB3	1.88	0.55
1:D:337:PHE:HD1	1:D:337:PHE:C	2.14	0.55
1:A:273:ARG:NH2	1:A:377:ALA:HB1	2.22	0.55
1:B:334:MSE:HE2	1:B:338:LYS:HD3	1.89	0.55
1:C:35:ILE:HD12	1:C:70:PRO:HG2	1.87	0.55
1:D:177:ASP:O	1:D:182:ILE:HD13	2.07	0.55
1:D:458:HIS:O	1:D:462:MSE:SE	2.74	0.55
1:A:44:ILE:O	1:A:53:ARG:HG2	2.06	0.55
1:D:337:PHE:C	1:D:337:PHE:CD1	2.85	0.55
1:B:334:MSE:HE2	1:B:338:LYS:HD2	1.89	0.55
1:D:126:LYS:O	1:D:126:LYS:HE2	2.06	0.55
1:D:160:ARG:HG2	1:D:161:ALA:N	2.18	0.55
1:A:189:TRP:CE3	1:A:248:VAL:HG11	2.42	0.54
1:B:405:ILE:HG12	1:B:410:TRP:CE3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:GLU:CB	1:C:342:PRO:HD3	2.37	0.54
1:A:259:ARG:O	1:A:263:GLU:HG3	2.07	0.54
1:B:463:PHE:O	1:B:467:VAL:HB	2.06	0.54
1:C:21:PHE:CD1	1:C:75:PHE:HE1	2.25	0.54
1:C:39:ASP:HA	1:C:42:GLU:HB2	1.89	0.54
1:C:159:GLY:N	1:C:165:LYS:HD3	2.22	0.54
1:C:334:MSE:HE2	1:C:338:LYS:CD	2.38	0.54
1:D:208:LEU:HD23	1:D:235:ILE:HA	1.88	0.54
1:D:529:PHE:HB3	1:D:532:PHE:CZ	2.42	0.54
1:A:395:PHE:O	1:A:397:VAL:N	2.40	0.54
1:D:190:LEU:HD13	1:D:203:LEU:HD22	1.90	0.54
1:A:211:LEU:CD1	1:A:239:LEU:HD23	2.37	0.54
1:A:342:PRO:O	1:A:343:LYS:HB3	2.07	0.54
1:B:166:SER:OG	1:B:250:ASP:OD1	2.26	0.54
1:C:368:PRO:HD3	1:D:279:ASN:O	2.06	0.54
1:D:233:ARG:HG3	1:D:233:ARG:HH11	1.72	0.54
1:D:342:PRO:HD2	1:D:347:LYS:HG3	1.89	0.54
1:B:414:ILE:HG21	1:B:430:VAL:HG13	1.90	0.54
1:C:128:MSE:SE	1:C:167:VAL:CG2	3.06	0.54
1:D:264:LEU:HD12	1:D:266:LEU:HD11	1.90	0.54
1:D:301:PHE:CE1	1:D:305:TYR:HE1	2.26	0.54
1:B:35:ILE:O	1:B:64:GLN:HB2	2.08	0.54
1:C:188:VAL:HB	1:C:247:PHE:CE1	2.42	0.54
1:D:189:TRP:CZ3	1:D:248:VAL:HG11	2.43	0.54
1:A:207:ILE:HD11	1:A:249:PHE:CE1	2.42	0.54
1:B:40:HIS:O	1:B:43:LEU:HB2	2.08	0.54
1:B:255:GLU:O	1:B:259:ARG:HG3	2.07	0.54
1:C:235:ILE:O	1:C:239:LEU:HB2	2.08	0.54
1:A:406:PRO:CA	1:A:453:THR:HG22	2.37	0.54
1:B:310:PRO:HA	1:B:345:PHE:HE1	1.72	0.54
1:A:127:GLN:CD	1:A:174:SER:HB3	2.33	0.54
1:A:452:LEU:H	1:A:452:LEU:CD2	2.17	0.54
1:D:364:GLU:CB	1:D:373:SER:HB3	2.33	0.54
1:A:233:ARG:HH11	1:A:233:ARG:CG	2.20	0.53
1:B:10:LEU:HB3	1:B:58:LEU:HD22	1.90	0.53
1:C:139:ARG:HH21	1:C:143:LYS:HE3	1.73	0.53
2:G:752:PHE:O	2:G:753:MSE:HG2	2.08	0.53
1:C:214:GLU:N	1:C:214:GLU:CD	2.66	0.53
1:C:395:PHE:HD2	1:C:415:PRO:HD3	1.74	0.53
1:D:237:ASN:C	1:D:239:LEU:H	2.16	0.53
1:A:382:VAL:O	1:A:385:LEU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:VAL:HB	1:B:247:PHE:CD1	2.43	0.53
1:C:253:VAL:HG11	1:C:380:ARG:HD3	1.90	0.53
1:C:527:GLU:C	1:C:530:PRO:HD3	2.33	0.53
1:A:465:LYS:HD3	1:A:466:HIS:HE1	1.72	0.53
1:D:395:PHE:O	1:D:397:VAL:N	2.42	0.53
1:B:128:MSE:HB2	1:B:171:GLN:NE2	2.23	0.53
1:B:159:GLY:N	1:B:165:LYS:HD3	2.23	0.53
1:B:521:GLU:C	1:B:523:VAL:H	2.16	0.53
1:D:447:LYS:HE3	1:D:450:PRO:HD2	1.91	0.53
1:A:90:TYR:CE2	1:A:106:ILE:HD11	2.38	0.53
1:C:313:GLU:O	1:C:316:GLU:HG3	2.09	0.53
1:D:188:VAL:HB	1:D:247:PHE:HD1	1.74	0.53
1:D:477:ILE:HG21	1:D:544:LYS:HG3	1.91	0.53
1:A:207:ILE:HD11	1:A:249:PHE:HE1	1.73	0.53
1:A:331:ALA:HB2	4:A:602:ATP:H5'1	1.88	0.53
1:B:50:ARG:CA	1:B:53:ARG:HH21	2.21	0.53
1:B:155:LEU:HB3	1:B:269:LEU:HD23	1.91	0.53
1:C:33:LYS:HD3	1:C:70:PRO:HG3	1.89	0.53
1:C:452:LEU:H	1:C:452:LEU:HD23	1.72	0.53
1:D:30:LEU:C	1:D:36:PHE:HB2	2.34	0.53
1:D:359:GLY:N	1:D:466:HIS:NE2	2.56	0.53
1:A:326:SER:O	1:A:328:GLY:N	2.42	0.53
1:B:109:GLN:C	1:B:111:SER:H	2.17	0.53
1:C:240:ILE:HG13	1:C:241:ASP:N	2.24	0.53
1:D:206:ASP:O	1:D:210:MSE:HG2	2.09	0.53
1:C:157:LEU:HD11	1:C:168:ILE:HG22	1.91	0.53
1:D:10:LEU:HB3	1:D:58:LEU:HD22	1.91	0.53
1:D:532:PHE:C	1:D:534:GLN:H	2.17	0.53
1:B:2:LEU:HB2	1:B:7:CYS:SG	2.49	0.53
1:D:23:PRO:HG2	1:D:53:ARG:C	2.33	0.53
1:A:444:LEU:O	1:A:445:SER:HB2	2.09	0.52
1:A:7:CYS:SG	1:A:62:ARG:HD3	2.48	0.52
1:A:210:MSE:HE1	1:B:233:ARG:HD3	1.91	0.52
1:C:327:SER:O	1:C:459:ILE:HD11	2.08	0.52
1:D:248:VAL:HG22	1:D:269:LEU:HB3	1.92	0.52
1:A:72:ILE:C	1:A:74:PHE:H	2.17	0.52
1:A:155:LEU:HB3	1:A:269:LEU:HD23	1.91	0.52
1:C:406:PRO:HA	1:C:453:THR:HG22	1.90	0.52
1:D:393:LEU:HD23	1:D:393:LEU:O	2.10	0.52
1:A:170:SER:O	1:A:174:SER:HB2	2.09	0.52
1:B:108:PRO:O	1:B:109:GLN:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:GLU:O	1:B:391:SER:HB3	2.10	0.52
1:C:230:VAL:O	1:C:234:MSE:HB2	2.09	0.52
1:A:166:SER:OG	1:A:250:ASP:OD1	2.28	0.52
1:A:527:GLU:OE1	1:A:527:GLU:N	2.41	0.52
1:B:105:VAL:HG22	1:B:110:PHE:CE2	2.44	0.52
1:B:230:VAL:HG12	1:B:234:MSE:HE2	1.91	0.52
1:B:383:GLU:HG2	2:F:753:MSE:HG2	1.90	0.52
1:B:411:SER:HA	1:B:430:VAL:HG21	1.91	0.52
1:C:47:MSE:HE2	1:C:52:GLU:HG2	1.91	0.52
1:A:72:ILE:HG23	1:A:84:ALA:HB1	1.90	0.52
1:A:93:PHE:CE2	1:A:104:VAL:HG11	2.45	0.52
1:C:163:SER:C	1:C:330:PRO:HG2	2.34	0.52
1:A:359:GLY:N	1:A:466:HIS:NE2	2.58	0.52
1:A:464:LEU:O	1:A:468:VAL:HG22	2.10	0.52
1:B:49:THR:HG22	1:B:50:ARG:N	2.24	0.52
1:B:452:LEU:HD23	1:B:452:LEU:H	1.75	0.52
1:A:37:THR:H	1:A:40:HIS:HB2	1.74	0.52
1:A:187:ILE:HD12	1:A:246:LEU:O	2.10	0.52
1:B:273:ARG:CZ	1:B:380:ARG:HH21	2.22	0.52
1:B:273:ARG:NE	4:B:602:ATP:O3G	2.41	0.52
1:C:7:CYS:SG	1:C:62:ARG:HD3	2.50	0.52
1:C:214:GLU:CD	1:C:214:GLU:H	2.17	0.52
1:C:230:VAL:HG12	1:C:234:MSE:HE3	1.91	0.52
1:A:195:THR:O	1:A:254:GLN:NE2	2.43	0.52
1:C:397:VAL:C	1:C:399:MSE:H	2.18	0.52
1:C:456:ILE:HG13	1:C:460:ILE:CG2	2.40	0.52
1:C:461:HIS:O	1:C:464:LEU:N	2.43	0.52
1:A:188:VAL:HB	1:A:247:PHE:CE1	2.45	0.51
1:C:23:PRO:O	1:C:27:LEU:HG	2.09	0.51
1:C:230:VAL:CG1	1:C:234:MSE:HE3	2.40	0.51
1:D:216:ASP:HA	1:D:219:ASN:HB2	1.92	0.51
1:A:376:MSE:O	1:A:379:GLN:HB3	2.09	0.51
1:B:8:ARG:O	1:B:12:THR:OG1	2.12	0.51
1:B:481:GLU:HA	1:B:484:LEU:HG	1.92	0.51
1:C:47:MSE:HB2	1:C:53:ARG:CG	2.38	0.51
1:C:195:THR:O	1:C:254:GLN:NE2	2.44	0.51
1:C:247:PHE:HE2	1:C:266:LEU:HD22	1.75	0.51
1:C:529:PHE:N	1:C:530:PRO:HD3	2.26	0.51
1:A:159:GLY:N	1:A:165:LYS:HD3	2.25	0.51
1:C:148:CYS:SG	1:C:183:ASN:ND2	2.81	0.51
1:C:401:PRO:HB2	1:C:458:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:LEU:O	1:C:460:ILE:HG21	2.10	0.51
1:D:341:GLU:CB	1:D:342:PRO:HD3	2.40	0.51
1:B:399:MSE:O	1:B:539:PHE:CZ	2.64	0.51
1:C:9:ALA:HB2	1:C:90:TYR:CD1	2.46	0.51
1:C:122:GLY:HA3	1:C:187:ILE:HG23	1.92	0.51
1:B:177:ASP:O	1:B:182:ILE:HD13	2.10	0.51
1:B:395:PHE:CD2	1:B:415:PRO:HD3	2.46	0.51
1:C:314:LYS:HA	1:C:317:ASP:HB2	1.93	0.51
1:A:250:ASP:OD1	1:A:271:THR:OG1	2.25	0.51
1:B:343:LYS:O	1:B:343:LYS:HG2	2.09	0.51
1:D:43:LEU:HD23	1:D:60:ILE:HD11	1.92	0.51
1:D:413:VAL:HG23	1:D:414:ILE:HD12	1.92	0.51
1:A:131:TYR:CD1	1:A:131:TYR:C	2.89	0.51
1:A:272:THR:OG1	1:A:273:ARG:N	2.43	0.51
1:B:32:GLY:C	1:B:34:ASN:H	2.19	0.51
1:C:410:TRP:CZ3	1:C:454:PHE:HB2	2.46	0.51
1:D:269:LEU:HD22	1:D:270:VAL:H	1.76	0.51
1:D:326:SER:O	1:D:328:GLY:N	2.44	0.51
1:D:390:ARG:HH11	2:H:753:MSE:SE	2.44	0.51
1:A:255:GLU:CA	1:A:277:ILE:HG22	2.40	0.51
1:B:334:MSE:HE3	1:B:337:PHE:HB2	1.93	0.51
1:B:410:TRP:CD1	1:B:414:ILE:HD13	2.45	0.51
1:C:72:ILE:HG21	1:C:88:GLU:HG3	1.91	0.51
1:C:364:GLU:HB3	1:C:373:SER:HB3	1.93	0.51
1:C:484:LEU:HD21	1:C:533:MSE:CG	2.41	0.51
1:D:142:LYS:O	1:D:146:GLU:HG3	2.10	0.51
1:A:92:ASP:C	1:A:94:ALA:H	2.19	0.51
1:A:248:VAL:HG22	1:A:269:LEU:HB3	1.92	0.51
1:B:37:THR:OG1	1:B:40:HIS:ND1	2.33	0.51
1:B:342:PRO:O	1:B:343:LYS:HB3	2.10	0.51
1:B:391:SER:OG	1:B:415:PRO:HG2	2.11	0.51
1:D:59:ARG:NH1	1:D:63:ARG:HH22	2.08	0.51
1:B:30:LEU:HD13	1:B:36:PHE:CE1	2.46	0.51
1:C:292:SER:HB3	1:C:328:GLY:HA3	1.92	0.51
1:D:527:GLU:C	1:D:530:PRO:HD3	2.36	0.51
1:A:335:MSE:HE3	1:A:364:GLU:HA	1.93	0.50
1:C:117:ARG:HH21	1:C:120:LEU:HD23	1.76	0.50
1:D:180:ILE:HD12	1:D:187:ILE:HB	1.91	0.50
1:D:385:LEU:HD22	1:D:389:ASP:HB3	1.93	0.50
1:A:4:GLU:OE2	1:A:267:ARG:NH2	2.44	0.50
1:A:415:PRO:O	1:A:416:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:HIS:O	1:B:44:ILE:HG13	2.10	0.50
1:C:36:PHE:HD2	1:C:40:HIS:HB3	1.76	0.50
1:C:269:LEU:HD22	1:C:270:VAL:H	1.76	0.50
1:A:264:LEU:HB2	1:A:266:LEU:HG	1.94	0.50
1:B:334:MSE:CE	1:B:337:PHE:HB2	2.41	0.50
1:B:473:ILE:CG2	1:B:547:ALA:HB2	2.41	0.50
1:C:411:SER:OG	1:C:430:VAL:HG21	2.12	0.50
1:B:43:LEU:O	1:B:47:MSE:SE	2.80	0.50
1:C:399:MSE:HE1	1:C:409:LEU:O	2.11	0.50
1:D:32:GLY:C	1:D:34:ASN:H	2.20	0.50
1:C:165:LYS:HG2	1:C:290:VAL:HG21	1.93	0.50
1:C:415:PRO:O	1:C:416:VAL:HG13	2.11	0.50
1:D:250:ASP:OD1	1:D:271:THR:OG1	2.27	0.50
1:D:400:PRO:HB2	1:D:403:VAL:HB	1.94	0.50
1:A:177:ASP:O	1:A:182:ILE:HD13	2.12	0.50
1:A:197:PRO:HD2	1:A:198:LYS:HE2	1.92	0.50
1:B:255:GLU:HB3	1:B:277:ILE:HG22	1.93	0.50
1:C:23:PRO:HG2	1:C:53:ARG:CB	2.42	0.50
1:D:40:HIS:O	1:D:44:ILE:HG13	2.11	0.50
1:D:315:GLU:HB3	1:D:345:PHE:CE2	2.46	0.50
1:A:99:ASP:C	1:A:101:LEU:N	2.70	0.50
1:C:50:ARG:HE	1:C:54:ILE:HD11	1.76	0.50
1:D:226:VAL:HG11	1:D:234:MSE:HE1	1.94	0.50
1:C:233:ARG:HH11	1:C:233:ARG:CG	2.25	0.50
1:A:99:ASP:C	1:A:101:LEU:H	2.19	0.49
1:A:379:GLN:O	1:A:383:GLU:HG3	2.12	0.49
1:B:88:GLU:O	1:B:91:ILE:HG22	2.11	0.49
1:B:466:HIS:ND1	1:B:466:HIS:N	2.59	0.49
1:C:204:PHE:C	1:C:231:LEU:HD21	2.37	0.49
1:A:273:ARG:NE	4:A:602:ATP:O3G	2.39	0.49
1:A:406:PRO:HD3	1:A:524:ILE:HD11	1.93	0.49
1:B:189:TRP:CE3	1:B:248:VAL:HG11	2.47	0.49
1:D:135:TYR:CE1	1:D:139:ARG:HD2	2.47	0.49
1:D:247:PHE:CE2	1:D:266:LEU:HD13	2.48	0.49
1:A:324:GLU:HG3	1:A:458:HIS:CD2	2.47	0.49
1:B:9:ALA:HB2	1:B:90:TYR:CE1	2.47	0.49
1:B:318:VAL:HG12	1:B:348:MSE:HE3	1.95	0.49
1:B:359:GLY:N	1:B:466:HIS:NE2	2.59	0.49
1:C:322:THR:OG1	1:C:348:MSE:SE	2.79	0.49
1:C:410:TRP:CD1	1:C:414:ILE:HD13	2.46	0.49
1:D:135:TYR:CZ	1:D:139:ARG:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:MSE:HG3	1:D:410:TRP:CE2	2.47	0.49
1:A:150:LEU:HD13	1:A:153:PHE:HB3	1.94	0.49
1:A:165:LYS:HG2	1:A:290:VAL:HG21	1.93	0.49
1:A:529:PHE:HB3	1:A:532:PHE:CE2	2.46	0.49
1:C:157:LEU:HD11	1:C:168:ILE:CG2	2.41	0.49
1:D:342:PRO:CD	1:D:347:LYS:HG3	2.42	0.49
1:A:171:GLN:O	1:A:175:LYS:N	2.45	0.49
1:A:379:GLN:HE22	2:E:754:GLY:N	2.11	0.49
1:B:17:LEU:HD23	1:B:21:PHE:CD2	2.46	0.49
1:C:111:SER:C	1:C:113:GLN:H	2.20	0.49
1:C:447:LYS:CE	1:C:450:PRO:HD2	2.40	0.49
1:D:21:PHE:H	1:D:50:ARG:NH2	2.10	0.49
1:A:214:GLU:HG3	1:B:237:ASN:ND2	2.27	0.49
1:A:351:LEU:HD13	1:A:363:VAL:HG23	1.94	0.49
1:B:153:PHE:CE2	1:B:267:ARG:HB3	2.47	0.49
1:B:404:ASP:OD2	1:B:453:THR:OG1	2.27	0.49
1:C:189:TRP:CE3	1:C:248:VAL:HG21	2.47	0.49
1:C:296:ASP:O	1:C:299:TYR:HB2	2.13	0.49
1:C:403:VAL:HG12	1:C:405:ILE:HG22	1.93	0.49
1:D:467:VAL:HG13	2:H:750:PHE:HD1	1.78	0.49
1:B:233:ARG:HH11	1:B:233:ARG:CG	2.25	0.49
1:B:383:GLU:HG2	2:F:753:MSE:HB3	1.93	0.49
1:C:484:LEU:CD1	1:C:533:MSE:HG2	2.37	0.49
1:C:388:GLU:HG2	1:C:433:ARG:HH21	1.77	0.49
1:C:526:PRO:HG2	1:C:529:PHE:CD2	2.48	0.49
1:A:8:ARG:HG2	1:A:8:ARG:NH1	2.25	0.49
1:C:190:LEU:CD1	1:C:207:ILE:HG13	2.35	0.49
1:C:466:HIS:ND1	1:C:466:HIS:N	2.61	0.49
1:D:465:LYS:HD3	1:D:466:HIS:CE1	2.48	0.49
1:A:143:LYS:HB3	1:A:147:MSE:CE	2.42	0.49
1:A:200:THR:HG21	1:A:256:GLU:HB3	1.95	0.49
1:A:205:THR:HA	1:A:231:LEU:HD11	1.94	0.49
1:A:374:LEU:HD13	1:A:374:LEU:O	2.13	0.49
1:A:435:LYS:HZ1	1:A:446:GLY:HA3	1.77	0.49
1:B:127:GLN:HA	1:B:170:SER:OG	2.13	0.49
1:B:190:LEU:HD13	1:B:203:LEU:HD22	1.95	0.49
1:B:326:SER:O	1:B:328:GLY:N	2.46	0.49
1:C:303:GLU:HA	1:C:309:MSE:HE1	1.94	0.49
1:D:395:PHE:C	1:D:397:VAL:H	2.21	0.49
1:A:275:VAL:HG12	1:A:275:VAL:O	2.12	0.48
1:A:368:PRO:HD3	1:B:279:ASN:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:HH11	1:B:63:ARG:HH22	1.60	0.48
1:B:319:LEU:HA	1:B:348:MSE:HE1	1.95	0.48
1:B:529:PHE:N	1:B:530:PRO:HD3	2.28	0.48
2:F:749:MSE:O	2:F:750:PHE:HB2	2.13	0.48
1:C:349:ALA:HA	1:C:352:ASN:HB2	1.94	0.48
1:A:160:ARG:HD3	1:A:460:ILE:HD13	1.95	0.48
1:B:29:TYR:OH	1:B:33:LYS:HD2	2.13	0.48
1:B:141:ILE:HD12	1:B:175:LYS:NZ	2.28	0.48
1:B:154:PHE:CE2	1:B:262:GLN:HG3	2.49	0.48
1:B:487:ILE:O	1:B:531:LYS:NZ	2.46	0.48
1:C:128:MSE:HE3	1:D:282:SER:CB	2.43	0.48
1:C:262:GLN:O	1:C:262:GLN:HG2	2.12	0.48
1:B:355:LEU:HD21	1:B:363:VAL:HB	1.95	0.48
1:D:394:ALA:O	1:D:468:VAL:HG11	2.14	0.48
1:A:343:LYS:O	1:A:343:LYS:HG2	2.12	0.48
1:B:47:MSE:HB3	1:B:52:GLU:HB3	1.96	0.48
1:B:400:PRO:HA	1:B:401:PRO:HD3	1.73	0.48
1:C:188:VAL:HB	1:C:247:PHE:CD1	2.48	0.48
1:D:6:GLU:O	1:D:9:ALA:HB3	2.14	0.48
1:D:178:GLN:HB3	1:D:183:ASN:OD1	2.13	0.48
1:D:233:ARG:HH11	1:D:233:ARG:CG	2.27	0.48
1:A:315:GLU:HA	1:A:318:VAL:HG23	1.96	0.48
1:A:334:MSE:HA	1:A:334:MSE:CE	2.41	0.48
1:A:521:GLU:C	1:A:523:VAL:H	2.21	0.48
1:B:335:MSE:HE2	1:B:363:VAL:CG1	2.43	0.48
1:C:18:ILE:HD11	1:C:51:LEU:HD21	1.95	0.48
1:D:284:THR:O	1:D:285:CYS:C	2.57	0.48
1:D:335:MSE:HE2	1:D:363:VAL:CG1	2.43	0.48
1:A:72:ILE:CD1	1:A:87:LEU:HB2	2.42	0.48
1:B:165:LYS:HE3	1:B:272:THR:O	2.13	0.48
1:C:397:VAL:HG22	1:C:464:LEU:CB	2.40	0.48
1:C:406:PRO:CA	1:C:453:THR:HG22	2.44	0.48
1:C:434:LEU:HA	1:C:437:LEU:HB2	1.95	0.48
1:D:405:ILE:HG13	1:D:409:LEU:HB3	1.95	0.48
1:A:135:TYR:O	1:A:139:ARG:HG3	2.13	0.48
1:A:115:LEU:HD21	1:A:180:ILE:HB	1.94	0.48
1:A:215:ASP:O	1:A:216:ASP:HB2	2.14	0.48
1:A:395:PHE:O	1:A:398:VAL:HG22	2.13	0.48
1:A:529:PHE:N	1:A:530:PRO:HD3	2.29	0.48
1:B:17:LEU:O	1:B:54:ILE:HD13	2.13	0.48
1:B:187:ILE:HD13	1:B:246:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:PRO:O	1:D:416:VAL:HG23	2.13	0.48
1:A:23:PRO:HG2	1:A:53:ARG:CB	2.44	0.48
1:B:27:LEU:HD22	1:B:41:SER:HB2	1.96	0.48
1:C:189:TRP:CE3	1:C:248:VAL:HG11	2.49	0.48
1:C:326:SER:O	1:C:327:SER:C	2.55	0.48
1:D:133:ARG:CZ	1:D:293:LEU:HD23	2.43	0.48
1:D:466:HIS:ND1	1:D:466:HIS:N	2.62	0.48
1:B:157:LEU:HD23	1:B:288:ILE:O	2.14	0.48
1:C:453:THR:HG21	1:C:524:ILE:HD12	1.96	0.48
1:D:22:GLU:OE1	1:D:53:ARG:NH1	2.47	0.48
1:B:165:LYS:HG2	1:B:290:VAL:CG2	2.39	0.47
1:B:200:THR:HG21	1:B:256:GLU:HB3	1.95	0.47
1:B:341:GLU:CB	1:B:342:PRO:HD3	2.44	0.47
1:C:7:CYS:O	1:C:11:SER:HB2	2.14	0.47
1:C:36:PHE:CD2	1:C:40:HIS:HB3	2.48	0.47
1:C:315:GLU:HA	1:C:318:VAL:HG23	1.96	0.47
1:C:400:PRO:HB2	1:C:403:VAL:HB	1.95	0.47
1:C:543:LEU:HD23	1:C:543:LEU:HA	1.69	0.47
1:D:367:THR:HG23	1:D:369:TYR:HB3	1.94	0.47
1:D:410:TRP:HD1	1:D:414:ILE:HD13	1.79	0.47
1:A:37:THR:O	1:A:40:HIS:HB2	2.14	0.47
1:B:460:ILE:HD12	1:B:460:ILE:HA	1.76	0.47
1:D:158:HIS:NE2	1:D:289:GLU:HB2	2.29	0.47
1:D:302:LEU:CD1	1:D:319:LEU:HD21	2.45	0.47
1:D:398:VAL:HG11	1:D:477:ILE:N	2.29	0.47
1:C:165:LYS:HG2	1:C:290:VAL:CG2	2.43	0.47
1:D:21:PHE:CE2	1:D:23:PRO:HG3	2.50	0.47
1:A:178:GLN:HA	1:A:182:ILE:HD13	1.97	0.47
1:A:361:VAL:HG13	1:A:364:GLU:OE1	2.14	0.47
1:A:410:TRP:CZ3	1:A:454:PHE:HB2	2.49	0.47
1:A:444:LEU:HD12	1:A:444:LEU:HA	1.80	0.47
1:B:240:ILE:HG13	1:B:241:ASP:N	2.30	0.47
1:B:399:MSE:CE	1:B:410:TRP:HA	2.44	0.47
1:B:534:GLN:O	1:B:537:GLN:HB2	2.14	0.47
1:C:189:TRP:CD2	1:C:248:VAL:HG11	2.50	0.47
1:D:426:LEU:HB3	1:D:428:ASP:OD2	2.14	0.47
1:B:383:GLU:HG2	2:F:753:MSE:CB	2.44	0.47
1:B:171:GLN:O	1:B:175:LYS:HB2	2.15	0.47
1:B:374:LEU:HD13	1:B:378:LEU:HG	1.96	0.47
1:B:459:ILE:H	1:B:459:ILE:HG13	1.44	0.47
1:C:130:CYS:HB2	1:C:305:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:LEU:O	1:C:393:LEU:HD23	2.14	0.47
1:D:529:PHE:N	1:D:530:PRO:HD3	2.29	0.47
1:A:158:HIS:NE2	1:A:289:GLU:HB2	2.29	0.47
1:C:255:GLU:HA	1:C:277:ILE:HG22	1.97	0.47
1:C:354:LYS:O	1:C:358:ARG:HB2	2.15	0.47
1:B:192:ASP:OD2	1:B:257:THR:OG1	2.21	0.47
1:B:385:LEU:HD22	1:B:389:ASP:HB2	1.97	0.47
1:B:465:LYS:HD3	1:B:466:HIS:CE1	2.50	0.47
1:D:44:ILE:HD13	1:D:57:PHE:HD1	1.79	0.47
1:D:319:LEU:HD12	1:D:345:PHE:CZ	2.50	0.47
1:C:134:GLU:O	1:C:135:TYR:C	2.58	0.47
1:C:407:VAL:HG22	1:C:454:PHE:HE1	1.80	0.47
1:D:257:THR:HG22	1:D:258:ILE:N	2.30	0.47
1:A:326:SER:C	1:A:459:ILE:HG12	2.39	0.46
1:A:335:MSE:HE2	1:A:363:VAL:CG1	2.44	0.46
1:B:56:ASN:O	1:B:60:ILE:HB	2.14	0.46
1:B:109:GLN:C	1:B:111:SER:N	2.69	0.46
1:B:397:VAL:O	1:B:461:HIS:NE2	2.45	0.46
1:B:537:GLN:O	1:B:538:LYS:C	2.56	0.46
1:C:72:ILE:C	1:C:74:PHE:H	2.23	0.46
1:C:379:GLN:O	1:C:383:GLU:HG3	2.14	0.46
1:D:1:MSE:HA	1:D:62:ARG:O	2.15	0.46
1:D:116:ASP:O	1:D:120:LEU:HB3	2.16	0.46
1:D:133:ARG:O	1:D:137:VAL:HG23	2.14	0.46
1:D:398:VAL:HG11	1:D:476:GLY:C	2.39	0.46
1:A:347:LYS:O	1:A:347:LYS:HD3	2.15	0.46
1:B:8:ARG:HD3	1:B:90:TYR:OH	2.15	0.46
1:C:187:ILE:HD13	1:C:246:LEU:HB3	1.97	0.46
1:C:302:LEU:CD1	1:C:319:LEU:HD21	2.45	0.46
1:C:478:SER:O	1:C:482:GLN:HG2	2.15	0.46
1:D:2:LEU:CD1	1:D:62:ARG:HE	2.28	0.46
1:D:110:PHE:HD1	1:D:110:PHE:HA	1.57	0.46
1:D:127:GLN:HB3	1:D:170:SER:O	2.15	0.46
1:A:249:PHE:HE2	1:A:261:ALA:HB2	1.81	0.46
1:C:74:PHE:CD2	1:C:74:PHE:C	2.92	0.46
1:C:378:LEU:HA	1:C:378:LEU:HD23	1.70	0.46
1:D:283:GLN:C	1:D:285:CYS:N	2.71	0.46
1:D:399:MSE:HG3	1:D:410:TRP:CZ2	2.51	0.46
1:D:461:HIS:O	1:D:464:LEU:N	2.48	0.46
1:B:26:ALA:HB2	1:B:74:PHE:CZ	2.49	0.46
1:B:128:MSE:CG	1:B:167:VAL:HG22	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:ASN:O	1:B:479:ILE:HG13	2.16	0.46
1:C:301:PHE:HE1	1:C:305:TYR:HE2	1.63	0.46
1:D:187:ILE:CD1	1:D:246:LEU:HB3	2.45	0.46
1:D:227:THR:HB	1:D:229:VAL:HG12	1.97	0.46
1:D:355:LEU:HD21	1:D:363:VAL:HB	1.97	0.46
1:A:471:GLN:HG3	1:D:471:GLN:HE21	1.80	0.46
1:B:434:LEU:HD22	1:B:444:LEU:CD2	2.46	0.46
1:D:144:LEU:HB2	1:D:179:LEU:HD21	1.98	0.46
1:D:237:ASN:C	1:D:239:LEU:N	2.74	0.46
1:A:21:PHE:CE1	1:A:75:PHE:HE1	2.34	0.46
1:C:160:ARG:HB3	1:C:163:SER:HB3	1.97	0.46
1:C:342:PRO:O	1:C:343:LYS:HB3	2.16	0.46
1:C:449:MSE:HE3	1:C:450:PRO:HA	1.97	0.46
1:A:482:GLN:C	1:A:484:LEU:H	2.21	0.46
1:C:19:HIS:HD2	1:D:1:MSE:SE	2.48	0.46
1:C:319:LEU:HD12	1:C:345:PHE:CZ	2.50	0.46
1:D:397:VAL:C	1:D:399:MSE:H	2.23	0.46
1:A:21:PHE:CD1	1:A:75:PHE:HE1	2.34	0.46
1:A:22:GLU:HG3	1:A:24:ARG:H	1.81	0.46
1:A:189:TRP:CD1	1:A:189:TRP:C	2.94	0.46
1:A:395:PHE:C	1:A:397:VAL:H	2.23	0.46
1:B:126:LYS:HE2	1:B:126:LYS:O	2.16	0.46
1:B:173:LEU:HD23	1:B:179:LEU:HD23	1.98	0.46
1:C:21:PHE:CD1	1:C:75:PHE:CE1	3.04	0.46
1:C:165:LYS:HE3	1:C:272:THR:O	2.16	0.46
1:C:219:ASN:O	1:C:221:PRO:HD3	2.16	0.46
1:D:118:LYS:HD3	1:D:180:ILE:HG22	1.98	0.46
1:D:207:ILE:HD11	1:D:249:PHE:HE1	1.80	0.46
1:B:49:THR:HG22	1:B:51:LEU:H	1.80	0.46
1:B:69:GLY:C	1:B:71:LEU:H	2.24	0.46
1:C:216:ASP:N	1:C:218:LEU:HD23	2.31	0.46
1:D:135:TYR:O	1:D:139:ARG:HG3	2.16	0.46
1:D:187:ILE:HD13	1:D:246:LEU:HD23	1.97	0.46
1:D:399:MSE:HE3	1:D:410:TRP:CG	2.51	0.46
1:B:26:ALA:HA	1:B:74:PHE:CE1	2.51	0.45
1:C:218:LEU:HG	1:C:219:ASN:N	2.32	0.45
1:D:100:LEU:HD12	1:D:100:LEU:HA	1.83	0.45
1:D:334:MSE:HE3	1:D:334:MSE:HA	1.98	0.45
1:A:79:ASN:HD22	1:B:36:PHE:N	2.14	0.45
1:A:237:ASN:C	1:A:239:LEU:H	2.24	0.45
1:A:257:THR:HG22	1:A:258:ILE:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ARG:O	1:B:165:LYS:NZ	2.48	0.45
1:B:274:ASP:OD2	1:B:440:ARG:NH1	2.49	0.45
1:D:399:MSE:HE3	1:D:410:TRP:CD1	2.50	0.45
1:B:226:VAL:HG11	1:B:234:MSE:CE	2.46	0.45
1:C:189:TRP:CD1	1:C:189:TRP:C	2.95	0.45
1:D:197:PRO:HD2	1:D:198:LYS:HE2	1.97	0.45
1:A:390:ARG:HE	1:A:390:ARG:HB2	1.10	0.45
1:A:393:LEU:HD23	1:A:393:LEU:C	2.41	0.45
1:B:393:LEU:HB2	1:B:437:LEU:HD11	1.97	0.45
1:B:408:LYS:HD2	1:B:408:LYS:HA	1.66	0.45
1:C:141:ILE:HD12	1:C:175:LYS:HZ2	1.81	0.45
1:C:237:ASN:C	1:C:239:LEU:H	2.23	0.45
1:C:318:VAL:HG13	1:C:349:ALA:HB2	1.97	0.45
1:A:397:VAL:HG21	1:A:468:VAL:HG21	1.98	0.45
1:C:35:ILE:O	1:C:64:GLN:HB3	2.16	0.45
1:A:17:LEU:HD23	1:A:21:PHE:CD2	2.51	0.45
1:A:163:SER:O	1:A:330:PRO:HG2	2.17	0.45
1:A:437:LEU:HD22	1:A:437:LEU:HA	1.70	0.45
1:B:23:PRO:HG2	1:B:53:ARG:O	2.15	0.45
1:B:49:THR:HG22	1:B:50:ARG:H	1.82	0.45
1:B:385:LEU:HD22	1:B:389:ASP:CB	2.47	0.45
1:C:37:THR:H	1:C:40:HIS:HB2	1.81	0.45
1:C:477:ILE:HD13	1:C:544:LYS:HG3	1.98	0.45
1:D:255:GLU:HB3	1:D:277:ILE:HG22	1.97	0.45
1:D:331:ALA:HB2	4:D:602:ATP:H5'1	1.98	0.45
1:D:395:PHE:C	1:D:397:VAL:N	2.74	0.45
1:D:414:ILE:HG21	1:D:430:VAL:HG13	1.99	0.45
1:C:388:GLU:CD	1:C:388:GLU:H	2.24	0.45
1:D:247:PHE:HE2	1:D:266:LEU:HD22	1.81	0.45
1:D:259:ARG:O	1:D:263:GLU:HG3	2.16	0.45
1:D:319:LEU:HD12	1:D:345:PHE:HE1	1.80	0.45
2:H:752:PHE:HB3	2:H:753:MSE:C	2.42	0.45
1:A:405:ILE:HG12	1:A:410:TRP:CZ3	2.51	0.45
1:B:30:LEU:HD23	1:B:30:LEU:HA	1.75	0.45
1:B:367:THR:HG23	1:B:369:TYR:HB3	1.99	0.45
1:C:38:GLU:O	1:C:38:GLU:CG	2.65	0.45
1:C:333:LEU:O	1:C:336:PHE:HB2	2.16	0.45
1:D:192:ASP:OD2	1:D:257:THR:OG1	2.21	0.45
1:D:521:GLU:C	1:D:523:VAL:H	2.24	0.45
1:A:25:ASP:HB3	1:A:78:ASN:ND2	2.32	0.45
1:B:394:ALA:O	1:B:397:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:GLU:HG2	1:C:69:GLY:N	2.29	0.45
1:C:359:GLY:N	1:C:466:HIS:NE2	2.65	0.45
1:C:382:VAL:HA	1:C:385:LEU:HD12	1.98	0.45
1:D:387:ASP:HA	1:D:390:ARG:HH21	1.81	0.45
1:B:189:TRP:CZ3	1:B:248:VAL:HG11	2.52	0.45
1:B:252:VAL:CG2	1:B:257:THR:HG21	2.47	0.45
1:B:255:GLU:CB	1:B:277:ILE:HG22	2.46	0.45
1:D:143:LYS:O	1:D:147:MSE:HG3	2.17	0.45
1:D:329:ASN:HA	1:D:330:PRO:HD2	1.70	0.45
1:D:463:PHE:O	1:D:467:VAL:HB	2.17	0.45
1:A:235:ILE:O	1:A:239:LEU:HB2	2.18	0.44
1:A:467:VAL:O	2:E:751:ASN:HB2	2.16	0.44
1:C:258:ILE:CG2	1:C:280:ALA:HB3	2.47	0.44
1:C:331:ALA:HB2	4:C:602:ATP:H5'1	1.99	0.44
1:D:491:ASN:HD21	1:D:531:LYS:HE3	1.82	0.44
1:A:461:HIS:O	1:A:464:LEU:N	2.50	0.44
1:B:253:VAL:HG11	1:B:380:ARG:HD3	1.99	0.44
1:B:405:ILE:HA	1:B:406:PRO:HD3	1.59	0.44
1:B:434:LEU:HD22	1:B:444:LEU:HD23	1.99	0.44
1:C:240:ILE:HG13	1:C:241:ASP:OD1	2.18	0.44
1:C:302:LEU:HD13	1:C:319:LEU:HD21	1.98	0.44
1:D:469:ASP:HB2	2:H:749:MSE:HA	1.99	0.44
1:B:397:VAL:HG22	1:B:464:LEU:HB3	1.97	0.44
1:C:33:LYS:NZ	1:C:73:ASP:OD2	2.50	0.44
1:C:484:LEU:HD21	1:C:533:MSE:HG2	1.98	0.44
1:A:408:LYS:HD2	1:A:408:LYS:HA	1.83	0.44
1:B:410:TRP:CZ3	1:B:454:PHE:HB2	2.52	0.44
1:C:136:HIS:O	1:C:137:VAL:C	2.57	0.44
1:D:252:VAL:CG2	1:D:257:THR:HG21	2.47	0.44
1:A:140:VAL:HG12	1:A:144:LEU:HD12	1.99	0.44
1:B:429:GLU:O	1:B:429:GLU:HG3	2.18	0.44
1:D:527:GLU:HA	1:D:530:PRO:HG3	1.99	0.44
1:A:397:VAL:HG22	1:A:464:LEU:CB	2.48	0.44
1:B:307:MSE:HA	1:B:308:PRO:HD3	1.79	0.44
1:A:11:SER:OG	1:A:185:ASP:OD2	2.28	0.44
1:A:79:ASN:ND2	1:B:36:PHE:O	2.51	0.44
1:A:168:ILE:HD13	1:A:168:ILE:HG21	1.74	0.44
1:A:212:LYS:HA	1:A:212:LYS:HE2	2.00	0.44
1:A:247:PHE:CD2	1:A:266:LEU:HD13	2.53	0.44
1:B:44:ILE:O	1:B:53:ARG:HG2	2.18	0.44
1:B:147:MSE:O	1:B:150:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:HIS:CE1	1:C:289:GLU:HB2	2.53	0.44
1:C:274:ASP:C	1:C:274:ASP:OD1	2.60	0.44
1:D:335:MSE:SE	1:D:373:SER:HA	2.68	0.44
1:D:399:MSE:CE	1:D:410:TRP:HA	2.48	0.44
1:A:79:ASN:ND2	1:B:36:PHE:N	2.65	0.44
1:C:337:PHE:CD1	1:C:337:PHE:C	2.95	0.44
1:D:2:LEU:HD12	1:D:7:CYS:SG	2.58	0.44
1:D:17:LEU:HD23	1:D:21:PHE:CD2	2.53	0.44
1:D:27:LEU:HD22	1:D:41:SER:HA	2.00	0.44
1:D:322:THR:OG1	1:D:348:MSE:SE	2.86	0.44
1:A:243:PRO:O	1:A:244:ASN:C	2.61	0.44
1:A:395:PHE:C	1:A:397:VAL:N	2.76	0.44
1:D:534:GLN:O	1:D:537:GLN:HB2	2.17	0.44
1:A:120:LEU:HD13	1:B:265:ARG:HB2	1.99	0.43
1:B:134:GLU:O	1:B:135:TYR:C	2.61	0.43
1:D:148:CYS:HB3	1:D:183:ASN:HB3	2.00	0.43
1:D:393:LEU:HD21	1:D:464:LEU:HD21	2.00	0.43
1:C:75:PHE:HB3	1:C:83:LEU:HB2	1.99	0.43
1:C:126:LYS:HE2	1:C:126:LYS:O	2.18	0.43
1:C:136:HIS:HB3	1:C:168:ILE:HD13	1.99	0.43
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.61	0.43
2:H:750:PHE:O	2:H:751:ASN:ND2	2.23	0.43
1:A:160:ARG:HG2	1:A:161:ALA:N	2.28	0.43
1:A:469:ASP:HB2	2:E:749:MSE:HA	1.99	0.43
1:B:2:LEU:HB2	1:B:7:CYS:HG	1.84	0.43
1:B:395:PHE:C	1:B:397:VAL:H	2.26	0.43
1:C:46:LYS:H	1:C:46:LYS:HG3	1.66	0.43
1:D:127:GLN:CD	1:D:174:SER:HB3	2.42	0.43
1:D:166:SER:HA	1:D:271:THR:HG21	2.01	0.43
1:D:207:ILE:O	1:D:210:MSE:HB2	2.17	0.43
1:D:434:LEU:HD22	1:D:444:LEU:HD21	2.00	0.43
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.82	0.43
1:A:405:ILE:HA	1:A:406:PRO:HD3	1.69	0.43
1:C:131:TYR:CD1	1:C:131:TYR:C	2.96	0.43
1:C:329:ASN:HA	1:C:330:PRO:HD2	1.84	0.43
1:D:315:GLU:HA	1:D:318:VAL:HG23	1.99	0.43
1:D:482:GLN:N	1:D:482:GLN:OE1	2.51	0.43
1:B:189:TRP:CD1	1:B:189:TRP:C	2.96	0.43
1:B:386:SER:OG	1:B:388:GLU:OE1	2.36	0.43
1:D:4:GLU:O	1:D:8:ARG:HG3	2.18	0.43
1:D:21:PHE:HD2	1:D:54:ILE:HG12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472:THR:HG21	2:H:749:MSE:HE2	2.00	0.43
1:A:111:SER:C	1:A:113:GLN:H	2.26	0.43
1:B:382:VAL:O	1:B:385:LEU:HB2	2.18	0.43
1:C:111:SER:HB3	1:C:113:GLN:HG2	2.00	0.43
1:C:178:GLN:O	1:C:182:ILE:HB	2.19	0.43
2:G:750:PHE:HB2	2:G:753:MSE:HE2	2.00	0.43
1:D:157:LEU:HD11	1:D:168:ILE:CG2	2.48	0.43
1:D:301:PHE:O	1:D:304:ALA:HB3	2.18	0.43
1:D:349:ALA:HA	1:D:352:ASN:HB2	2.01	0.43
1:A:36:PHE:HE2	1:A:44:ILE:HD12	1.82	0.43
1:B:295:ILE:HG23	1:B:323:ILE:HG21	1.99	0.43
1:B:340:CYS:SG	1:B:348:MSE:HG2	2.58	0.43
1:B:393:LEU:HD21	1:B:464:LEU:HD21	2.01	0.43
1:D:126:LYS:HE2	1:D:126:LYS:HB3	1.74	0.43
1:D:207:ILE:HG22	1:D:208:LEU:N	2.33	0.43
1:D:257:THR:HG22	1:D:258:ILE:HD12	2.01	0.43
1:B:160:ARG:HG3	1:B:441:GLY:O	2.17	0.43
1:B:190:LEU:HD23	1:B:190:LEU:HA	1.81	0.43
1:B:207:ILE:HG22	1:B:208:LEU:N	2.34	0.43
1:B:527:GLU:C	1:B:530:PRO:HD3	2.44	0.43
1:C:248:VAL:HG22	1:C:269:LEU:HB3	2.00	0.43
1:C:408:LYS:HE2	1:C:427:ASP:HB2	2.01	0.43
1:D:315:GLU:HB3	1:D:345:PHE:CD2	2.53	0.43
1:D:460:ILE:HD12	1:D:460:ILE:HA	1.77	0.43
1:B:329:ASN:HA	1:B:330:PRO:HD2	1.84	0.43
1:C:157:LEU:HD23	1:C:288:ILE:O	2.19	0.43
1:D:405:ILE:HG12	1:D:410:TRP:CE3	2.53	0.43
1:D:527:GLU:OE1	1:D:527:GLU:N	2.51	0.43
1:A:40:HIS:CD2	1:A:64:GLN:NE2	2.87	0.43
1:A:307:MSE:HE1	1:A:348:MSE:HG3	2.01	0.43
1:B:477:ILE:HD13	1:B:544:LYS:HG3	2.00	0.43
1:C:111:SER:O	1:C:113:GLN:N	2.51	0.43
1:C:258:ILE:HG22	1:C:280:ALA:HB3	2.01	0.43
1:C:459:ILE:HG13	1:C:459:ILE:H	1.32	0.43
1:C:461:HIS:C	1:C:463:PHE:N	2.74	0.43
1:C:485:LEU:HD12	1:C:486:GLU:H	1.83	0.43
1:D:255:GLU:O	1:D:259:ARG:HG3	2.19	0.43
1:D:358:ARG:C	1:D:466:HIS:NE2	2.77	0.43
1:A:24:ARG:HE	1:A:53:ARG:NH1	2.17	0.42
1:A:455:LYS:HG2	1:A:456:ILE:N	2.33	0.42
1:A:532:PHE:C	1:A:534:GLN:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:GLU:CB	1:C:373:SER:HB3	2.48	0.42
1:A:72:ILE:HG21	1:A:88:GLU:CG	2.42	0.42
1:A:133:ARG:HH12	1:A:290:VAL:HG12	1.83	0.42
1:A:136:HIS:O	1:A:139:ARG:N	2.53	0.42
1:A:157:LEU:HD22	1:A:290:VAL:HG22	2.00	0.42
1:A:449:MSE:HE3	1:A:449:MSE:HB2	1.76	0.42
1:C:273:ARG:NH2	1:C:377:ALA:HB1	2.34	0.42
1:C:354:LYS:HE2	1:D:429:GLU:OE1	2.19	0.42
1:A:435:LYS:HZ3	1:A:446:GLY:HA3	1.83	0.42
1:A:543:LEU:HA	1:A:543:LEU:HD23	1.77	0.42
1:B:34:ASN:O	1:B:35:ILE:HG13	2.19	0.42
1:B:46:LYS:O	1:B:47:MSE:SE	2.87	0.42
1:B:308:PRO:CG	1:B:343:LYS:HD3	2.49	0.42
1:B:532:PHE:C	1:B:534:GLN:H	2.27	0.42
1:C:334:MSE:HE3	1:C:334:MSE:HA	2.00	0.42
1:C:393:LEU:HB2	1:C:437:LEU:HD11	2.01	0.42
1:C:482:GLN:C	1:C:484:LEU:H	2.26	0.42
1:D:139:ARG:HH21	1:D:143:LYS:HE3	1.83	0.42
1:A:167:VAL:HG12	1:A:168:ILE:N	2.34	0.42
1:B:157:LEU:HD22	1:B:290:VAL:HG22	2.01	0.42
1:B:158:HIS:O	1:B:158:HIS:ND1	2.52	0.42
1:B:347:LYS:O	1:B:347:LYS:HD3	2.19	0.42
1:C:237:ASN:HD22	1:C:237:ASN:HA	1.67	0.42
1:C:465:LYS:HB3	1:C:466:HIS:ND1	2.35	0.42
1:D:301:PHE:HE1	1:D:305:TYR:HE1	1.65	0.42
1:D:318:VAL:O	1:D:321:LYS:HB3	2.19	0.42
1:D:438:SER:O	1:D:442:ALA:HA	2.18	0.42
1:D:529:PHE:HB3	1:D:532:PHE:CE1	2.55	0.42
1:D:530:PRO:HD2	1:D:531:LYS:HG3	2.00	0.42
1:A:124:VAL:HA	1:A:125:PRO:HD3	1.67	0.42
1:B:331:ALA:HB2	4:B:602:ATP:H5'1	2.00	0.42
1:C:38:GLU:O	1:C:38:GLU:HG2	2.20	0.42
1:C:72:ILE:HD11	1:C:87:LEU:HB2	2.01	0.42
1:C:113:GLN:H	1:C:113:GLN:HG2	1.66	0.42
1:C:325:LEU:HD12	1:C:352:ASN:OD1	2.20	0.42
1:C:538:LYS:C	1:C:540:TYR:H	2.27	0.42
1:D:105:VAL:HG22	1:D:110:PHE:CE2	2.55	0.42
1:A:21:PHE:CG	1:A:22:GLU:N	2.87	0.42
1:A:302:LEU:HD13	1:A:319:LEU:HD11	2.01	0.42
1:B:154:PHE:HE2	1:B:262:GLN:HG3	1.84	0.42
1:B:525:ARG:HD3	1:B:525:ARG:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ASP:OD1	1:C:96:ASN:ND2	2.48	0.42
1:D:39:ASP:O	1:D:43:LEU:HD13	2.20	0.42
1:D:49:THR:HG22	1:D:50:ARG:N	2.35	0.42
1:D:100:LEU:HB3	1:D:101:LEU:H	1.65	0.42
1:D:136:HIS:O	1:D:140:VAL:HG23	2.20	0.42
1:D:141:ILE:HD12	1:D:175:LYS:CE	2.48	0.42
1:A:525:ARG:HA	1:A:526:PRO:HD3	1.73	0.42
1:B:122:GLY:HA3	1:B:187:ILE:HG23	2.02	0.42
1:B:332:THR:HG23	1:B:374:LEU:HB2	2.00	0.42
1:C:60:ILE:HG23	1:C:64:GLN:HG3	2.01	0.42
1:C:395:PHE:O	1:C:398:VAL:HG22	2.20	0.42
1:C:525:ARG:HA	1:C:526:PRO:HD3	1.54	0.42
1:D:104:VAL:HG12	1:D:105:VAL:HG23	2.01	0.42
1:D:408:LYS:HD2	1:D:408:LYS:HA	1.76	0.42
1:A:204:PHE:O	1:A:231:LEU:HD21	2.20	0.42
1:A:235:ILE:HG21	1:A:235:ILE:HD13	1.78	0.42
1:C:2:LEU:HG	1:C:62:ARG:HA	2.02	0.42
1:C:4:GLU:OE2	1:C:267:ARG:NH2	2.53	0.42
1:D:302:LEU:HB3	1:D:307:MSE:HB3	2.01	0.42
1:A:142:LYS:HE2	1:A:146:GLU:OE2	2.20	0.42
1:C:192:ASP:O	1:C:193:SER:HB2	2.19	0.42
1:D:121:LEU:HD23	1:D:121:LEU:HA	1.64	0.42
1:A:24:ARG:HH21	1:A:53:ARG:NH1	2.18	0.42
1:A:117:ARG:HH21	1:A:120:LEU:CD2	2.29	0.42
1:A:135:TYR:CZ	1:A:139:ARG:HD2	2.55	0.42
1:A:479:ILE:HG23	1:A:483:ARG:HH22	1.84	0.42
1:A:527:GLU:C	1:A:530:PRO:HD3	2.45	0.42
2:E:752:PHE:N	2:E:752:PHE:CD1	2.88	0.42
1:B:2:LEU:HD12	1:B:7:CYS:SG	2.59	0.42
1:C:21:PHE:CG	1:C:22:GLU:N	2.88	0.42
1:C:319:LEU:HA	1:C:348:MSE:HE1	2.02	0.42
1:C:405:ILE:O	1:C:405:ILE:HG12	2.20	0.42
1:A:19:HIS:O	1:B:1:MSE:HG3	2.20	0.41
1:A:182:ILE:N	1:A:182:ILE:HD12	2.35	0.41
1:A:435:LYS:HD3	1:A:435:LYS:HA	1.90	0.41
1:B:313:GLU:O	1:B:316:GLU:HG3	2.20	0.41
1:D:27:LEU:CD1	1:D:45:SER:HB3	2.51	0.41
1:D:168:ILE:HA	1:D:171:GLN:HE21	1.85	0.41
1:A:63:ARG:HE	1:A:240:ILE:CD1	2.12	0.41
1:A:240:ILE:HG13	1:A:241:ASP:N	2.35	0.41
1:B:160:ARG:HG2	1:B:161:ALA:N	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:HD23	1:B:393:LEU:O	2.20	0.41
1:C:8:ARG:NH1	1:C:185:ASP:OD1	2.52	0.41
1:C:385:LEU:HD22	1:C:389:ASP:HB3	2.02	0.41
1:D:127:GLN:HB2	1:D:171:GLN:HA	2.01	0.41
1:D:235:ILE:HD13	1:D:235:ILE:HG21	1.73	0.41
1:D:325:LEU:HD23	1:D:325:LEU:HA	1.80	0.41
1:A:35:ILE:O	1:A:64:GLN:HB3	2.20	0.41
1:A:91:ILE:O	1:A:95:ILE:HG13	2.20	0.41
1:B:22:GLU:OE2	1:B:53:ARG:HD2	2.20	0.41
1:B:167:VAL:HG12	1:B:168:ILE:N	2.35	0.41
1:B:194:GLY:O	1:B:254:GLN:HG3	2.21	0.41
1:C:397:VAL:O	1:C:399:MSE:N	2.50	0.41
1:C:405:ILE:HA	1:C:406:PRO:HD3	1.78	0.41
1:C:434:LEU:HD22	1:C:444:LEU:HD23	2.02	0.41
1:D:2:LEU:N	1:D:2:LEU:HD23	2.35	0.41
1:D:335:MSE:CE	1:D:373:SER:HB2	2.49	0.41
1:D:481:GLU:HA	1:D:484:LEU:HG	2.02	0.41
1:A:327:SER:N	1:A:459:ILE:HG12	2.36	0.41
1:A:371:TYR:CD2	1:A:377:ALA:HB2	2.55	0.41
1:A:379:GLN:NE2	2:E:753:MSE:C	2.78	0.41
1:A:388:GLU:O	1:A:391:SER:HB3	2.20	0.41
1:B:283:GLN:C	1:B:285:CYS:H	2.28	0.41
1:B:395:PHE:O	1:B:397:VAL:N	2.54	0.41
1:B:405:ILE:HD13	1:B:405:ILE:HG21	1.69	0.41
1:D:242:ARG:HH11	1:D:242:ARG:HD2	1.65	0.41
1:D:247:PHE:CD2	1:D:266:LEU:HB3	2.55	0.41
1:D:366:ILE:H	1:D:366:ILE:CD1	2.16	0.41
1:D:385:LEU:HD11	1:D:393:LEU:HD12	2.01	0.41
1:D:434:LEU:HD22	1:D:444:LEU:CD2	2.50	0.41
1:A:38:GLU:O	1:A:42:GLU:HB2	2.20	0.41
1:A:157:LEU:HD22	1:A:290:VAL:CG2	2.50	0.41
1:A:332:THR:O	1:A:336:PHE:HB2	2.20	0.41
1:A:385:LEU:O	1:A:390:ARG:NH2	2.53	0.41
1:B:92:ASP:O	1:B:96:ASN:HB2	2.21	0.41
1:B:218:LEU:HG	1:B:219:ASN:N	2.36	0.41
1:B:330:PRO:HB3	4:B:602:ATP:N3	2.35	0.41
1:B:487:ILE:HA	1:B:490:ASN:OD1	2.20	0.41
1:C:34:ASN:O	1:C:35:ILE:HG13	2.21	0.41
1:C:426:LEU:HB3	1:C:428:ASP:OD1	2.20	0.41
1:D:157:LEU:HD22	1:D:290:VAL:CG2	2.50	0.41
1:D:190:LEU:HD12	1:D:207:ILE:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:LEU:HA	1:D:460:ILE:HG12	2.02	0.41
1:A:72:ILE:HD11	1:A:87:LEU:CB	2.47	0.41
1:A:459:ILE:HG13	1:A:459:ILE:H	1.46	0.41
1:B:256:GLU:O	1:B:257:THR:C	2.64	0.41
1:B:295:ILE:O	1:B:299:TYR:HD1	2.03	0.41
1:B:368:PRO:HB2	4:B:602:ATP:O2'	2.21	0.41
1:B:397:VAL:O	1:B:399:MSE:N	2.54	0.41
1:C:8:ARG:HG2	1:C:8:ARG:NH1	2.29	0.41
1:D:104:VAL:HB	1:D:105:VAL:H	1.63	0.41
1:A:188:VAL:HB	1:A:247:PHE:CD1	2.55	0.41
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.76	0.41
1:A:478:SER:HB3	1:D:548:CYS:SG	2.60	0.41
1:B:250:ASP:HA	1:B:271:THR:OG1	2.20	0.41
1:C:116:ASP:OD1	1:C:116:ASP:N	2.54	0.41
1:D:533:MSE:C	1:D:535:LEU:N	2.77	0.41
1:A:303:GLU:HA	1:A:309:MSE:HE1	2.03	0.41
1:B:113:GLN:O	1:B:117:ARG:N	2.53	0.41
1:C:99:ASP:C	1:C:101:LEU:H	2.28	0.41
1:C:371:TYR:CD2	1:C:377:ALA:HB2	2.56	0.41
1:C:426:LEU:HA	1:C:426:LEU:HD23	1.73	0.41
1:C:525:ARG:HD3	1:C:535:LEU:HD13	2.03	0.41
1:D:207:ILE:O	1:D:210:MSE:N	2.54	0.41
1:D:252:VAL:HG22	1:D:257:THR:HG21	2.02	0.41
1:A:2:LEU:HG	1:A:62:ARG:HA	2.03	0.41
1:A:165:LYS:H	1:A:165:LYS:HG3	1.58	0.41
1:A:254:GLN:C	1:A:256:GLU:H	2.28	0.41
1:A:379:GLN:NE2	2:E:754:GLY:N	2.69	0.41
1:A:413:VAL:HG23	1:A:414:ILE:HD12	2.03	0.41
1:A:429:GLU:OE2	1:A:433:ARG:NH1	2.54	0.41
1:A:471:GLN:HG3	1:D:471:GLN:NE2	2.35	0.41
1:B:32:GLY:C	1:B:34:ASN:N	2.79	0.41
1:B:135:TYR:CZ	1:B:139:ARG:HD2	2.56	0.41
1:B:158:HIS:ND1	1:B:158:HIS:C	2.79	0.41
1:B:188:VAL:HB	1:B:247:PHE:HD1	1.84	0.41
1:B:207:ILE:O	1:B:210:MSE:N	2.54	0.41
1:B:211:LEU:HD11	1:B:239:LEU:HD23	2.03	0.41
1:B:437:LEU:HD23	1:B:437:LEU:HA	1.81	0.41
1:B:481:GLU:O	1:B:484:LEU:HG	2.20	0.41
1:C:92:ASP:C	1:C:94:ALA:H	2.29	0.41
1:C:139:ARG:HD2	1:C:288:ILE:HG23	2.03	0.41
1:C:206:ASP:OD2	1:D:229:VAL:HG11	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:MSE:HE2	1:C:363:VAL:HG13	2.03	0.41
1:C:408:LYS:HD2	1:C:408:LYS:HA	1.74	0.41
1:C:456:ILE:HG12	1:C:457:ASP:O	2.21	0.41
1:D:43:LEU:HD12	1:D:43:LEU:HA	1.90	0.41
1:D:122:GLY:HA3	1:D:187:ILE:HG23	2.02	0.41
1:D:165:LYS:H	1:D:165:LYS:HG3	1.56	0.41
1:D:443:LEU:HD23	1:D:460:ILE:HD11	2.02	0.41
1:D:444:LEU:HB3	1:D:445:SER:H	1.66	0.41
1:A:72:ILE:HG23	1:A:72:ILE:HD12	1.85	0.41
1:A:78:ASN:OD1	1:B:37:THR:HG21	2.21	0.41
1:A:389:ASP:HB3	1:A:437:LEU:CD2	2.46	0.41
1:A:394:ALA:O	1:A:397:VAL:HG23	2.20	0.41
1:A:465:LYS:HB3	1:A:466:HIS:H	1.81	0.41
1:B:397:VAL:C	1:B:399:MSE:H	2.29	0.41
1:C:1:MSE:HE2	1:C:1:MSE:HB3	1.64	0.41
1:C:119:LEU:CB	1:D:265:ARG:HH12	2.34	0.41
1:C:197:PRO:HD2	1:C:198:LYS:CE	2.51	0.41
1:C:254:GLN:C	1:C:256:GLU:N	2.79	0.41
1:D:67:GLU:N	1:D:67:GLU:OE1	2.54	0.41
1:D:153:PHE:CE1	1:D:267:ARG:HB3	2.56	0.41
1:D:378:LEU:O	1:D:379:GLN:C	2.64	0.41
1:D:483:ARG:HA	1:D:486:GLU:HB2	2.03	0.41
1:A:142:LYS:O	1:A:146:GLU:HG3	2.20	0.40
1:A:395:PHE:CD2	1:A:415:PRO:HD3	2.56	0.40
1:B:180:ILE:HD12	1:B:187:ILE:HB	2.03	0.40
1:B:207:ILE:HD11	1:B:249:PHE:HE1	1.85	0.40
1:C:99:ASP:C	1:C:101:LEU:N	2.79	0.40
1:C:158:HIS:O	1:C:158:HIS:ND1	2.54	0.40
1:C:158:HIS:CD2	1:C:275:VAL:HG13	2.55	0.40
1:C:325:LEU:C	1:C:327:SER:H	2.28	0.40
1:C:349:ALA:O	1:C:352:ASN:HB2	2.20	0.40
1:C:416:VAL:HG12	1:C:429:GLU:HG2	2.02	0.40
1:C:465:LYS:HB3	1:C:466:HIS:H	1.80	0.40
1:C:469:ASP:N	2:G:749:MSE:O	2.46	0.40
1:D:39:ASP:OD1	1:D:39:ASP:N	2.52	0.40
1:D:44:ILE:HG12	1:D:56:ASN:HB3	2.03	0.40
1:D:335:MSE:HE3	1:D:373:SER:HB2	2.03	0.40
2:H:749:MSE:O	2:H:750:PHE:HB2	2.22	0.40
1:A:111:SER:O	1:A:113:GLN:N	2.54	0.40
1:A:201:PHE:CD1	1:A:201:PHE:C	3.00	0.40
1:A:296:ASP:O	1:A:299:TYR:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:VAL:HG11	1:A:476:GLY:HA3	2.03	0.40
1:A:485:LEU:HD12	1:A:486:GLU:OE2	2.21	0.40
1:B:155:LEU:HD23	1:B:155:LEU:HA	1.77	0.40
1:B:186:SER:OG	1:B:245:THR:HG23	2.22	0.40
1:B:273:ARG:NH2	1:B:380:ARG:HH21	2.20	0.40
1:B:521:GLU:HG3	1:B:523:VAL:H	1.86	0.40
1:C:327:SER:OG	1:C:458:HIS:HB2	2.21	0.40
1:C:521:GLU:C	1:C:523:VAL:H	2.28	0.40
1:D:524:ILE:HD12	1:D:525:ARG:H	1.86	0.40
1:A:157:LEU:HA	1:A:288:ILE:O	2.22	0.40
1:A:326:SER:O	1:A:327:SER:C	2.65	0.40
1:B:200:THR:O	1:B:200:THR:HG22	2.20	0.40
1:B:240:ILE:C	1:B:242:ARG:H	2.29	0.40
1:B:372:LYS:H	1:B:376:MSE:HE2	1.87	0.40
1:C:139:ARG:HD2	1:C:288:ILE:CG2	2.52	0.40
1:C:139:ARG:HD3	1:C:139:ARG:C	2.47	0.40
1:C:443:LEU:C	1:C:460:ILE:HG12	2.47	0.40
1:D:61:TYR:HE2	1:D:68:LEU:HD22	1.85	0.40
1:D:137:VAL:HG13	1:D:172:ALA:HB2	2.02	0.40
1:D:400:PRO:HG3	1:D:533:MSE:HE1	2.04	0.40
1:A:256:GLU:O	1:A:257:THR:C	2.64	0.40
1:A:313:GLU:O	1:A:316:GLU:HG3	2.21	0.40
1:A:439:LYS:HD2	1:A:439:LYS:HA	1.75	0.40
1:A:447:LYS:HE2	1:A:449:MSE:O	2.21	0.40
1:B:217:LEU:HD23	1:B:217:LEU:HA	1.89	0.40
1:B:234:MSE:O	1:B:237:ASN:HB2	2.22	0.40
1:C:117:ARG:HH12	1:D:240:ILE:HA	1.86	0.40
1:C:237:ASN:C	1:C:239:LEU:N	2.80	0.40
1:C:382:VAL:O	1:C:385:LEU:HB2	2.22	0.40
1:C:390:ARG:HE	1:C:390:ARG:HB2	1.56	0.40
1:D:204:PHE:N	1:D:204:PHE:CD1	2.88	0.40
1:D:406:PRO:CA	1:D:453:THR:HG22	2.47	0.40
1:D:474:ALA:HB2	1:D:547:ALA:CB	2.51	0.40
1:A:349:ALA:HA	1:A:352:ASN:HB2	2.04	0.40
1:B:20:ASP:O	1:B:21:PHE:HB2	2.22	0.40
1:B:39:ASP:O	1:B:43:LEU:HD22	2.22	0.40
1:B:187:ILE:HD12	1:B:246:LEU:O	2.21	0.40
1:B:322:THR:OG1	1:B:348:MSE:SE	2.90	0.40
1:C:72:ILE:CD1	1:C:87:LEU:HB2	2.52	0.40
1:C:378:LEU:O	1:C:379:GLN:C	2.64	0.40
1:D:276:GLU:C	1:D:278:SER:N	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:LEU:HD13	1:D:531:LYS:O	2.22	0.40
1:D:539:PHE:CZ	1:D:543:LEU:HD22	2.55	0.40

All (1) 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:C:2:LEU:O	1:D:113:GLN:NE2[4_555]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	504/549 (92%)	404 (80%)	77 (15%)	23 (5%)	2	15
1	B	505/549 (92%)	407 (81%)	73 (14%)	25 (5%)	1	13
1	C	504/549 (92%)	404 (80%)	76 (15%)	24 (5%)	2	14
1	D	505/549 (92%)	405 (80%)	77 (15%)	23 (5%)	2	15
2	E	4/8 (50%)	1 (25%)	2 (50%)	1 (25%)	0	0
2	F	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	G	3/8 (38%)	1 (33%)	0	2 (67%)	0	0
2	H	4/8 (50%)	1 (25%)	2 (50%)	1 (25%)	0	0
All	All	2032/2228 (91%)	1624 (80%)	308 (15%)	100 (5%)	1	13

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	A	341	GLU
1	A	398	VAL

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Mol	Chain	Res	Type
1	A	445	SER
1	A	486	GLU
2	E	751	ASN
1	B	109	GLN
1	B	127	GLN
1	B	284	THR
1	B	327	SER
1	B	341	GLU
1	B	398	VAL
1	B	445	SER
2	F	751	ASN
1	C	127	GLN
1	C	284	THR
1	C	327	SER
1	C	341	GLU
1	C	398	VAL
1	C	445	SER
2	G	751	ASN
1	D	35	ILE
1	D	127	GLN
1	D	284	THR
1	D	327	SER
1	D	341	GLU
1	D	398	VAL
1	D	445	SER
2	H	750	PHE
1	A	112	ARG
1	A	244	ASN
1	A	396	ALA
1	A	465	LYS
1	A	522	THR
1	B	244	ASN
1	B	396	ALA
1	B	465	LYS
1	C	112	ARG
1	C	244	ASN
1	C	396	ALA
1	C	465	LYS
1	C	522	THR
2	G	752	PHE
1	D	104	VAL
1	D	244	ASN

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Mol	Chain	Res	Type
1	D	396	ALA
1	D	465	LYS
1	D	522	THR
1	A	2	LEU
1	A	73	ASP
1	A	160	ARG
1	A	208	LEU
1	A	238	ALA
1	B	2	LEU
1	B	104	VAL
1	B	208	LEU
1	B	522	THR
1	C	2	LEU
1	C	73	ASP
1	C	208	LEU
1	C	238	ALA
1	D	160	ARG
1	D	208	LEU
1	D	238	ALA
1	A	284	THR
1	B	35	ILE
1	B	160	ARG
1	B	176	SER
1	C	160	ARG
1	C	485	LEU
1	C	486	GLU
1	D	52	GLU
1	D	111	SER
1	A	484	LEU
1	A	485	LEU
1	B	257	THR
1	B	328	GLY
1	C	484	LEU
1	D	34	ASN
1	D	257	THR
1	B	102	ARG
1	B	134	GLU
1	B	354	LYS
1	C	108	PRO
1	C	358	ARG
1	D	102	ARG
1	D	358	ARG

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Mol	Chain	Res	Type
1	B	106	ILE
1	B	311	VAL
1	D	311	VAL
1	A	70	PRO
1	A	108	PRO
1	A	328	GLY
1	B	70	PRO
1	C	70	PRO
1	C	311	VAL
1	A	311	VAL
1	C	35	ILE
1	A	35	ILE
1	D	328	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	462/483 (96%)	378 (82%)	84 (18%)	2	9
1	B	464/483 (96%)	377 (81%)	87 (19%)	1	9
1	C	462/483 (96%)	368 (80%)	94 (20%)	1	7
1	D	464/483 (96%)	365 (79%)	99 (21%)	1	6
2	E	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	F	5/5 (100%)	5 (100%)	0	100	100
2	G	5/5 (100%)	4 (80%)	1 (20%)	1	7
2	H	6/5 (120%)	5 (83%)	1 (17%)	2	11
All	All	1873/1952 (96%)	1505 (80%)	368 (20%)	1	8

All (368) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	4	GLU

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Mol	Chain	Res	Type
1	A	8	ARG
1	A	15	THR
1	A	17	LEU
1	A	43	LEU
1	A	46	LYS
1	A	47	MSE
1	A	51	LEU
1	A	52	GLU
1	A	67	GLU
1	A	68	LEU
1	A	77	TYR
1	A	82	HIS
1	A	95	ILE
1	A	100	LEU
1	A	113	GLN
1	A	115	LEU
1	A	117	ARG
1	A	126	LYS
1	A	128	MSE
1	A	130	CYS
1	A	131	TYR
1	A	132	ILE
1	A	148	CYS
1	A	155	LEU
1	A	157	LEU
1	A	167	VAL
1	A	174	SER
1	A	179	LEU
1	A	180	ILE
1	A	182	ILE
1	A	185	ASP
1	A	198	LYS
1	A	203	LEU
1	A	217	LEU
1	A	220	PHE
1	A	223	VAL
1	A	224	GLU
1	A	226	VAL
1	A	227	THR
1	A	233	ARG
1	A	239	LEU
1	A	241	ASP

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Mol	Chain	Res	Type
1	A	253	VAL
1	A	255	GLU
1	A	257	THR
1	A	264	LEU
1	A	269	LEU
1	A	272	THR
1	A	277	ILE
1	A	283	GLN
1	A	284	THR
1	A	286	GLU
1	A	296	ASP
1	A	316	GLU
1	A	332	THR
1	A	334	MSE
1	A	355	LEU
1	A	363	VAL
1	A	364	GLU
1	A	366	ILE
1	A	369	TYR
1	A	374	LEU
1	A	381	CYS
1	A	388	GLU
1	A	405	ILE
1	A	409	LEU
1	A	410	TRP
1	A	414	ILE
1	A	416	VAL
1	A	437	LEU
1	A	444	LEU
1	A	449	MSE
1	A	451	VAL
1	A	452	LEU
1	A	457	ASP
1	A	459	ILE
1	A	460	ILE
1	A	466	HIS
1	A	467	VAL
1	A	485	LEU
1	A	525	ARG
1	A	533	MSE
2	E	749	MSE
2	E	750	PHE

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Mol	Chain	Res	Type
1	B	1	MSE
1	B	4	GLU
1	B	15	THR
1	B	17	LEU
1	B	18	ILE
1	B	35	ILE
1	B	41	SER
1	B	43	LEU
1	B	46	LYS
1	B	51	LEU
1	B	52	GLU
1	B	64	GLN
1	B	67	GLU
1	B	68	LEU
1	B	77	TYR
1	B	97	GLU
1	B	99	ASP
1	B	104	VAL
1	B	109	GLN
1	B	112	ARG
1	B	116	ASP
1	B	117	ARG
1	B	126	LYS
1	B	128	MSE
1	B	130	CYS
1	B	131	TYR
1	B	148	CYS
1	B	155	LEU
1	B	157	LEU
1	B	160	ARG
1	B	167	VAL
1	B	174	SER
1	B	175	LYS
1	B	179	LEU
1	B	180	ILE
1	B	185	ASP
1	B	189	TRP
1	B	198	LYS
1	B	203	LEU
1	B	208	LEU
1	B	217	LEU
1	B	218	LEU

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Mol	Chain	Res	Type
1	B	220	PHE
1	B	223	VAL
1	B	226	VAL
1	B	227	THR
1	B	233	ARG
1	B	239	LEU
1	B	241	ASP
1	B	253	VAL
1	B	255	GLU
1	B	262	GLN
1	B	269	LEU
1	B	272	THR
1	B	277	ILE
1	B	284	THR
1	B	296	ASP
1	B	316	GLU
1	B	329	ASN
1	B	332	THR
1	B	355	LEU
1	B	363	VAL
1	B	364	GLU
1	B	366	ILE
1	B	369	TYR
1	B	374	LEU
1	B	381	CYS
1	B	382	VAL
1	B	388	GLU
1	B	404	ASP
1	B	405	ILE
1	B	409	LEU
1	B	410	TRP
1	B	414	ILE
1	B	416	VAL
1	B	437	LEU
1	B	444	LEU
1	B	451	VAL
1	B	452	LEU
1	B	457	ASP
1	B	459	ILE
1	B	460	ILE
1	B	462	MSE
1	B	466	HIS

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Mol	Chain	Res	Type
1	B	467	VAL
1	B	528	ASP
1	B	539	PHE
1	C	1	MSE
1	C	8	ARG
1	C	11	SER
1	C	15	THR
1	C	17	LEU
1	C	43	LEU
1	C	45	SER
1	C	46	LYS
1	C	47	MSE
1	C	51	LEU
1	C	52	GLU
1	C	67	GLU
1	C	68	LEU
1	C	77	TYR
1	C	78	ASN
1	C	79	ASN
1	C	82	HIS
1	C	99	ASP
1	C	100	LEU
1	C	109	GLN
1	C	111	SER
1	C	113	GLN
1	C	115	LEU
1	C	116	ASP
1	C	117	ARG
1	C	126	LYS
1	C	131	TYR
1	C	132	ILE
1	C	148	CYS
1	C	155	LEU
1	C	157	LEU
1	C	167	VAL
1	C	174	SER
1	C	176	SER
1	C	179	LEU
1	C	180	ILE
1	C	185	ASP
1	C	198	LYS
1	C	203	LEU

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Mol	Chain	Res	Type
1	C	217	LEU
1	C	220	PHE
1	C	223	VAL
1	C	226	VAL
1	C	227	THR
1	C	233	ARG
1	C	234	MSE
1	C	237	ASN
1	C	239	LEU
1	C	241	ASP
1	C	253	VAL
1	C	255	GLU
1	C	264	LEU
1	C	269	LEU
1	C	277	ILE
1	C	284	THR
1	C	286	GLU
1	C	296	ASP
1	C	316	GLU
1	C	319	LEU
1	C	326	SER
1	C	332	THR
1	C	336	PHE
1	C	345	PHE
1	C	355	LEU
1	C	360	LEU
1	C	363	VAL
1	C	366	ILE
1	C	369	TYR
1	C	374	LEU
1	C	381	CYS
1	C	387	ASP
1	C	388	GLU
1	C	390	ARG
1	C	405	ILE
1	C	409	LEU
1	C	410	TRP
1	C	414	ILE
1	C	416	VAL
1	C	437	LEU
1	C	444	LEU
1	C	451	VAL

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Mol	Chain	Res	Type
1	C	452	LEU
1	C	456	ILE
1	C	457	ASP
1	C	459	ILE
1	C	460	ILE
1	C	466	HIS
1	C	467	VAL
1	C	485	LEU
1	C	486	GLU
1	C	524	ILE
1	C	525	ARG
1	C	533	MSE
1	C	543	LEU
2	G	753	MSE
1	D	1	MSE
1	D	2	LEU
1	D	3	CYS
1	D	12	THR
1	D	17	LEU
1	D	18	ILE
1	D	35	ILE
1	D	39	ASP
1	D	43	LEU
1	D	46	LYS
1	D	51	LEU
1	D	52	GLU
1	D	64	GLN
1	D	68	LEU
1	D	71	LEU
1	D	77	TYR
1	D	82	HIS
1	D	93	PHE
1	D	99	ASP
1	D	100	LEU
1	D	110	PHE
1	D	116	ASP
1	D	117	ARG
1	D	126	LYS
1	D	128	MSE
1	D	130	CYS
1	D	131	TYR
1	D	148	CYS

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Mol	Chain	Res	Type
1	D	155	LEU
1	D	157	LEU
1	D	167	VAL
1	D	174	SER
1	D	176	SER
1	D	179	LEU
1	D	180	ILE
1	D	185	ASP
1	D	198	LYS
1	D	203	LEU
1	D	205	THR
1	D	212	LYS
1	D	217	LEU
1	D	218	LEU
1	D	220	PHE
1	D	223	VAL
1	D	224	GLU
1	D	226	VAL
1	D	227	THR
1	D	233	ARG
1	D	239	LEU
1	D	241	ASP
1	D	253	VAL
1	D	255	GLU
1	D	262	GLN
1	D	264	LEU
1	D	269	LEU
1	D	277	ILE
1	D	284	THR
1	D	286	GLU
1	D	296	ASP
1	D	309	MSE
1	D	316	GLU
1	D	319	LEU
1	D	332	THR
1	D	334	MSE
1	D	336	PHE
1	D	337	PHE
1	D	345	PHE
1	D	355	LEU
1	D	363	VAL
1	D	364	GLU

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Mol	Chain	Res	Type
1	D	366	ILE
1	D	369	TYR
1	D	374	LEU
1	D	381	CYS
1	D	382	VAL
1	D	387	ASP
1	D	388	GLU
1	D	404	ASP
1	D	405	ILE
1	D	409	LEU
1	D	410	TRP
1	D	414	ILE
1	D	416	VAL
1	D	439	LYS
1	D	444	LEU
1	D	451	VAL
1	D	452	LEU
1	D	456	ILE
1	D	457	ASP
1	D	459	ILE
1	D	460	ILE
1	D	466	HIS
1	D	467	VAL
1	D	482	GLN
1	D	491	ASN
1	D	525	ARG
1	D	538	LYS
1	D	539	PHE
1	D	548	CYS
2	H	751	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	78	ASN
1	A	79	ASN
1	A	136	HIS
1	A	219	ASN
1	A	244	ASN
1	A	379	GLN
1	B	14	HIS

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Mol	Chain	Res	Type
1	B	475	ASN
1	C	64	GLN
1	C	80	GLN
1	C	136	HIS
1	D	136	HIS
1	D	183	ASN
1	D	244	ASN
1	D	262	GLN
1	D	458	HIS
1	D	471	GLN
1	D	475	ASN
1	D	490	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
4	ATP	A	602	3	32,33,33	2.57	6 (18%)	48,52,52	1.91	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	B	602	3	32,33,33	1.85	7 (21%)	48,52,52	2.19	15 (31%)
4	ATP	D	602	3	32,33,33	2.53	8 (25%)	48,52,52	2.39	16 (33%)
4	ATP	C	602	3	32,33,33	1.96	7 (21%)	48,52,52	1.83	7 (14%)

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
4	ATP	A	602	3	-	1/22/38/38	0/3/3/3
4	ATP	B	602	3	-	4/22/38/38	0/3/3/3
4	ATP	D	602	3	-	3/22/38/38	0/3/3/3
4	ATP	C	602	3	-	1/22/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	ATP	PB-O3B	7.59	1.67	1.59
4	D	602	ATP	C5-C4	7.39	1.52	1.39
4	A	602	ATP	PB-O3A	7.38	1.67	1.59
4	C	602	ATP	C5-C4	6.46	1.50	1.39
4	D	602	ATP	PA-O3A	5.87	1.65	1.59
4	A	602	ATP	C5-C4	5.68	1.49	1.39
4	B	602	ATP	C5-C4	5.55	1.49	1.39
4	D	602	ATP	PB-O3A	5.30	1.65	1.59
4	C	602	ATP	PB-O3A	4.52	1.64	1.59
4	A	602	ATP	PA-O3A	4.47	1.64	1.59
4	B	602	ATP	C5-N7	-4.26	1.31	1.39
4	D	602	ATP	C5-C6	4.11	1.52	1.41
4	B	602	ATP	PB-O3A	3.93	1.63	1.59
4	D	602	ATP	C1'-N9	3.92	1.57	1.46
4	D	602	ATP	PB-O3B	3.76	1.63	1.59
4	C	602	ATP	PA-O3A	3.60	1.63	1.59
4	D	602	ATP	C8-N7	3.38	1.38	1.31
4	B	602	ATP	PB-O3B	3.33	1.63	1.59
4	D	602	ATP	C4-N3	3.32	1.40	1.34
4	A	602	ATP	C5-C6	3.25	1.50	1.41
4	C	602	ATP	C8-N7	3.10	1.37	1.31
4	B	602	ATP	PA-O3A	2.79	1.62	1.59
4	C	602	ATP	C5-C6	2.79	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	ATP	C1'-N9	2.79	1.54	1.46
4	A	602	ATP	C8-N7	2.77	1.37	1.31
4	B	602	ATP	C1'-N9	2.52	1.53	1.46
4	C	602	ATP	C4-N3	2.26	1.38	1.34
4	B	602	ATP	C8-N7	2.26	1.36	1.31

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	ATP	C5-C4-N3	-7.51	116.38	126.72
4	C	602	ATP	C5-C4-N3	-6.09	118.34	126.72
4	A	602	ATP	C5-C4-N3	-5.91	118.57	126.72
4	B	602	ATP	C5-C4-N3	-5.80	118.72	126.72
4	B	602	ATP	N3-C4-N9	5.66	136.79	127.17
4	B	602	ATP	N6-C6-N1	5.39	130.38	118.38
4	D	602	ATP	N3-C4-N9	5.23	136.06	127.17
4	D	602	ATP	O4'-C1'-N9	4.83	117.37	108.09
4	C	602	ATP	N3-C4-N9	4.79	135.31	127.17
4	D	602	ATP	C2-N3-C4	4.76	123.45	111.83
4	D	602	ATP	O2A-PA-O3A	4.44	119.28	107.27
4	B	602	ATP	O4'-C1'-N9	4.35	116.44	108.09
4	A	602	ATP	N3-C4-N9	4.30	134.48	127.17
4	D	602	ATP	N3-C2-N1	-4.27	122.12	128.58
4	C	602	ATP	N3-C2-N1	-4.15	122.31	128.58
4	C	602	ATP	C2-N3-C4	4.03	121.67	111.83
4	A	602	ATP	C2-N3-C4	3.94	121.45	111.83
4	D	602	ATP	C4-C5-N7	-3.68	106.38	110.58
4	A	602	ATP	N3-C2-N1	-3.67	123.02	128.58
4	A	602	ATP	C4-C5-N7	-3.53	106.55	110.58
4	B	602	ATP	O2G-PG-O1G	3.23	123.41	110.83
4	B	602	ATP	C2-N1-C6	3.17	123.93	118.73
4	B	602	ATP	C6-C5-C4	3.14	121.46	117.18
4	D	602	ATP	O4'-C1'-C2'	-3.12	99.95	106.62
4	D	602	ATP	O2'-C2'-C3'	-3.09	101.92	111.82
4	D	602	ATP	C2'-C3'-C4'	-3.08	96.66	102.61
4	C	602	ATP	O2A-PA-O3A	3.01	115.40	107.27
4	B	602	ATP	C5-C6-N6	-2.98	115.90	123.29
4	B	602	ATP	C4-N9-C1'	2.98	133.59	126.63
4	B	602	ATP	C2'-C1'-N9	-2.89	106.11	113.30
4	C	602	ATP	C2-N1-C6	2.81	123.34	118.73
4	B	602	ATP	N3-C2-N1	-2.77	124.38	128.58
4	B	602	ATP	C1'-N9-C8	-2.76	120.96	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	ATP	C2-N1-C6	2.60	123.01	118.73
4	A	602	ATP	C2-N1-C6	2.52	122.87	118.73
4	A	602	ATP	C6-C5-N7	2.51	136.93	132.09
4	A	602	ATP	O5'-C5'-C4'	-2.50	100.47	108.99
4	B	602	ATP	C2-N3-C4	2.43	117.77	111.83
4	B	602	ATP	C6-C5-N7	-2.34	127.57	132.09
4	A	602	ATP	C5-N7-C8	2.29	107.05	103.45
4	A	602	ATP	O4'-C1'-C2'	-2.29	101.72	106.62
4	C	602	ATP	O4'-C1'-C2'	-2.27	101.76	106.62
4	A	602	ATP	O3A-PB-O1B	-2.25	103.95	110.70
4	A	602	ATP	O2G-PG-O1G	2.19	119.38	110.83
4	D	602	ATP	C5-N7-C8	2.19	106.89	103.45
4	D	602	ATP	C6-C5-N7	2.18	136.29	132.09
4	D	602	ATP	O5'-PA-O1A	-2.15	100.43	108.94
4	B	602	ATP	O3A-PA-O1A	-2.07	104.47	110.70
4	D	602	ATP	O2B-PB-O1B	2.07	122.06	112.44
4	A	602	ATP	O2A-PA-O3A	2.05	112.81	107.27
4	D	602	ATP	C3'-C2'-C1'	2.02	105.29	101.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

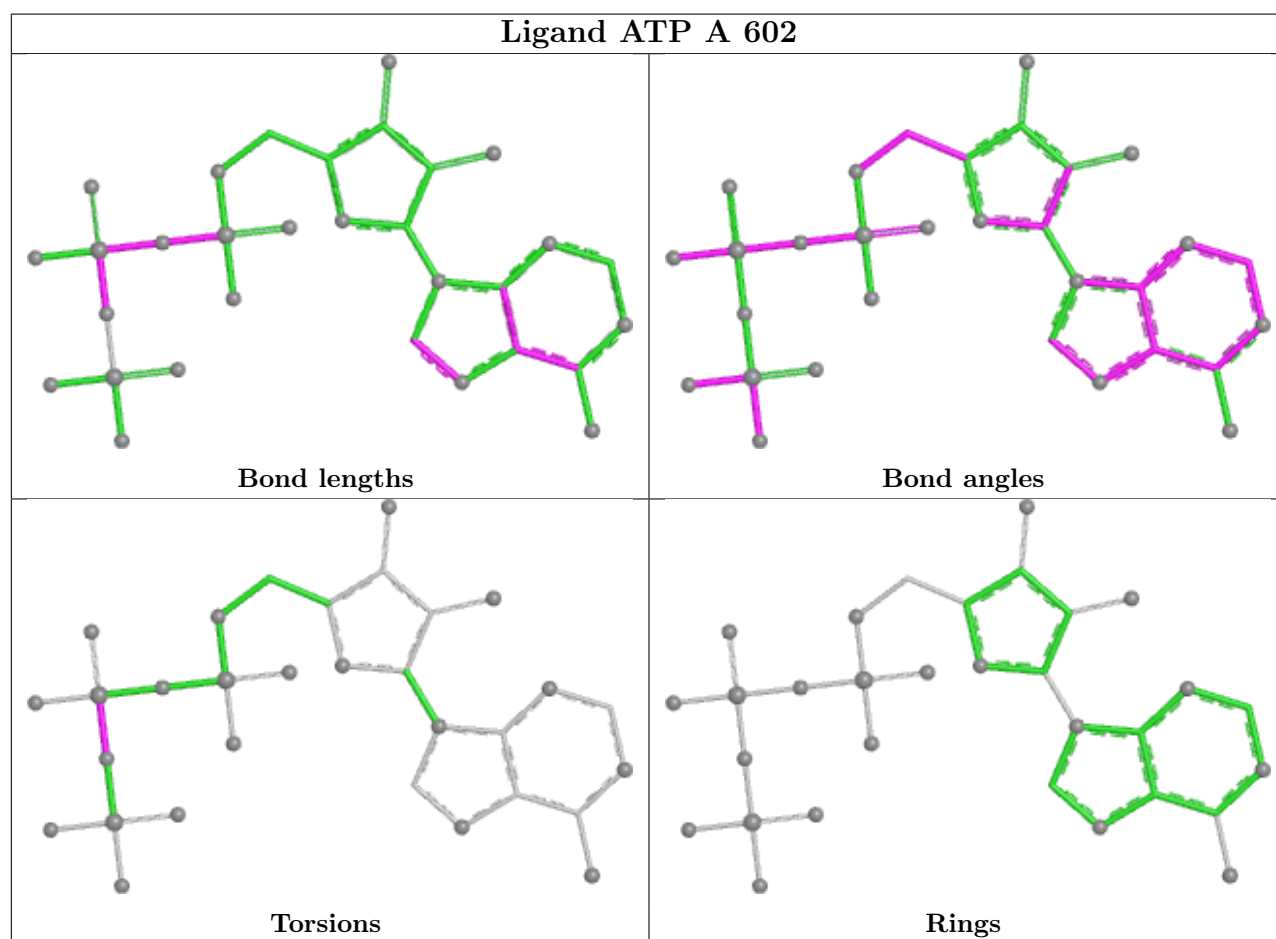
Mol	Chain	Res	Type	Atoms
4	B	602	ATP	O4'-C1'-N9-C8
4	B	602	ATP	O4'-C1'-N9-C4
4	D	602	ATP	O4'-C1'-N9-C8
4	D	602	ATP	O4'-C1'-N9-C4
4	A	602	ATP	PG-O3B-PB-O1B
4	B	602	ATP	PG-O3B-PB-O1B
4	C	602	ATP	PG-O3B-PB-O1B
4	B	602	ATP	PG-O3B-PB-O2B
4	D	602	ATP	C4'-C5'-O5'-PA

There are no ring outliers.

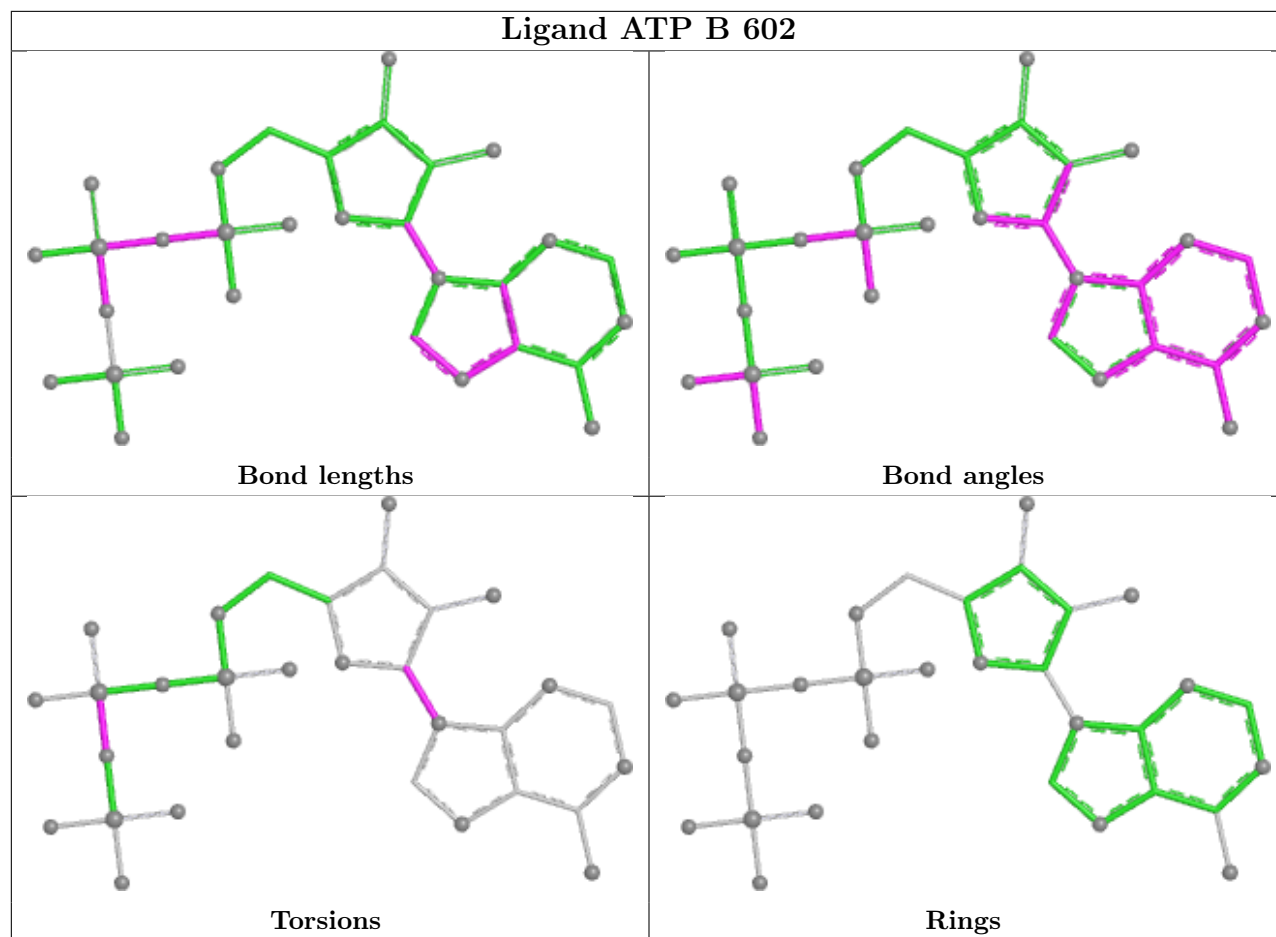
4 monomers are involved in 11 short contacts:

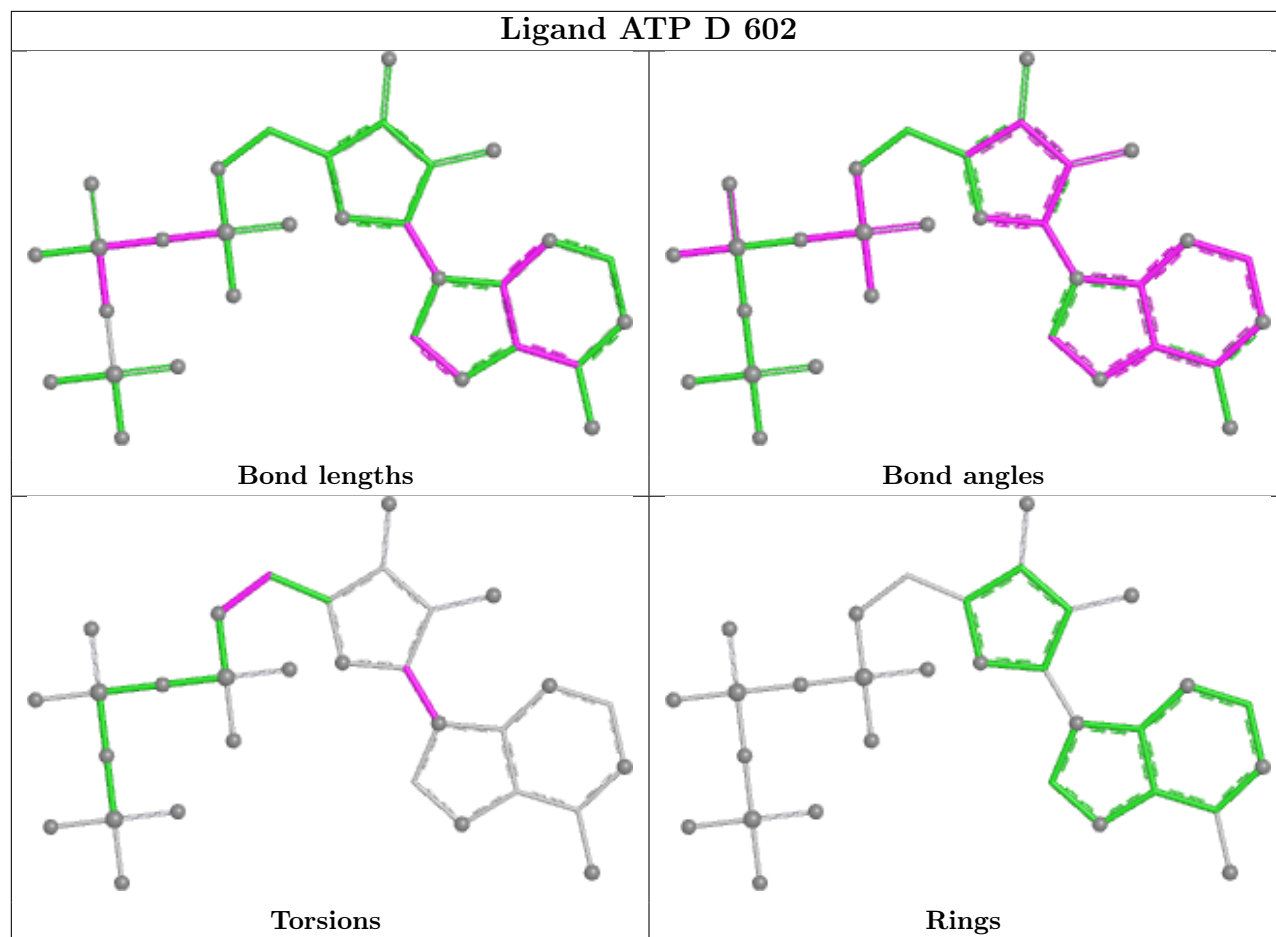
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	ATP	4	0
4	B	602	ATP	5	0
4	D	602	ATP	1	0
4	C	602	ATP	1	0

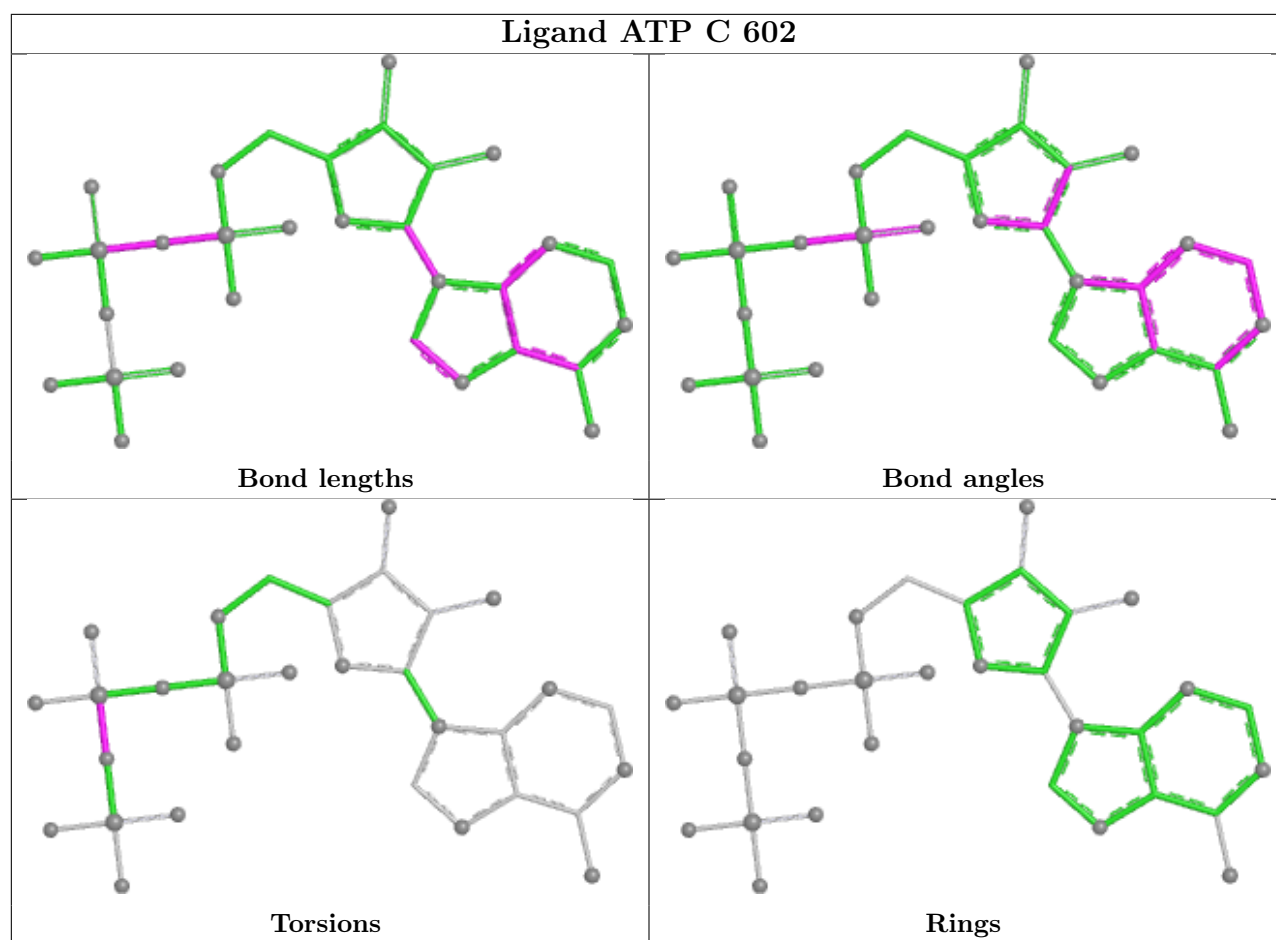
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand ATP B 602







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	493/549 (89%)	0.43	18 (3%) 45 28	45, 102, 177, 252	0
1	B	494/549 (89%)	0.54	27 (5%) 30 19	48, 98, 237, 286	0
1	C	493/549 (89%)	0.52	17 (3%) 48 30	62, 111, 177, 275	0
1	D	494/549 (89%)	0.61	23 (4%) 36 23	53, 111, 245, 281	0
2	E	4/8 (50%)	-0.29	0 100 100	81, 86, 86, 95	0
2	F	3/8 (37%)	0.17	0 100 100	74, 74, 78, 89	0
2	G	3/8 (37%)	-0.12	0 100 100	91, 91, 106, 110	0
2	H	4/8 (50%)	0.21	0 100 100	92, 108, 116, 126	0
All	All	1988/2228 (89%)	0.52	85 (4%) 40 24	45, 106, 214, 286	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	THR	4.2
1	B	51	LEU	3.8
1	B	10	LEU	3.8
1	A	539	PHE	3.7
1	D	51	LEU	3.6
1	D	70	PRO	3.2
1	A	159	GLY	3.2
1	B	71	LEU	3.1
1	A	77	TYR	3.1
1	D	410	TRP	3.0
1	A	290	VAL	3.0
1	C	77	TYR	3.0
1	B	337	PHE	3.0
1	D	91	ILE	2.9
1	A	29	TYR	2.8
1	B	115	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	68	LEU	2.7
1	D	341	GLU	2.7
1	D	283	GLN	2.6
1	C	66	SER	2.6
1	B	75	PHE	2.6
1	C	339	SER	2.6
1	C	283	GLN	2.6
1	B	107	ALA	2.6
1	C	398	VAL	2.6
1	D	252	VAL	2.6
1	D	61	TYR	2.5
1	A	16	ARG	2.5
1	C	51	LEU	2.5
1	A	454	PHE	2.5
1	B	299	TYR	2.5
1	B	484	LEU	2.5
1	A	301	PHE	2.5
1	B	170	SER	2.4
1	B	100	LEU	2.4
1	C	540	TYR	2.4
1	C	487	ILE	2.4
1	A	51	LEU	2.4
1	D	37	THR	2.4
1	B	58	LEU	2.3
1	B	18	ILE	2.3
1	A	325	LEU	2.3
1	D	176	SER	2.3
1	C	363	VAL	2.3
1	A	409	LEU	2.3
1	C	27	LEU	2.2
1	C	409	LEU	2.2
1	B	410	TRP	2.2
1	D	437	LEU	2.2
1	B	312	GLY	2.2
1	C	68	LEU	2.2
1	C	293	LEU	2.2
1	C	539	PHE	2.2
1	D	540	TYR	2.2
1	D	161	ALA	2.2
1	B	105	VAL	2.2
1	D	10	LEU	2.2
1	B	487	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	471	GLN	2.1
1	B	341	GLU	2.1
1	B	342	PRO	2.1
1	D	57	PHE	2.1
1	B	528	ASP	2.1
1	A	158	HIS	2.1
1	C	34	ASN	2.1
1	A	487	ILE	2.1
1	B	106	ILE	2.1
1	D	427	ASP	2.1
1	C	426	LEU	2.1
1	D	106	ILE	2.1
1	B	74	PHE	2.1
1	B	86	PHE	2.1
1	D	110	PHE	2.1
1	A	15	THR	2.0
1	D	103	PRO	2.0
1	B	68	LEU	2.0
1	D	121	LEU	2.0
1	A	91	ILE	2.0
1	D	487	ILE	2.0
1	A	76	ASN	2.0
1	B	540	TYR	2.0
1	D	274	ASP	2.0
1	C	32	GLY	2.0
1	B	398	VAL	2.0
1	A	18	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

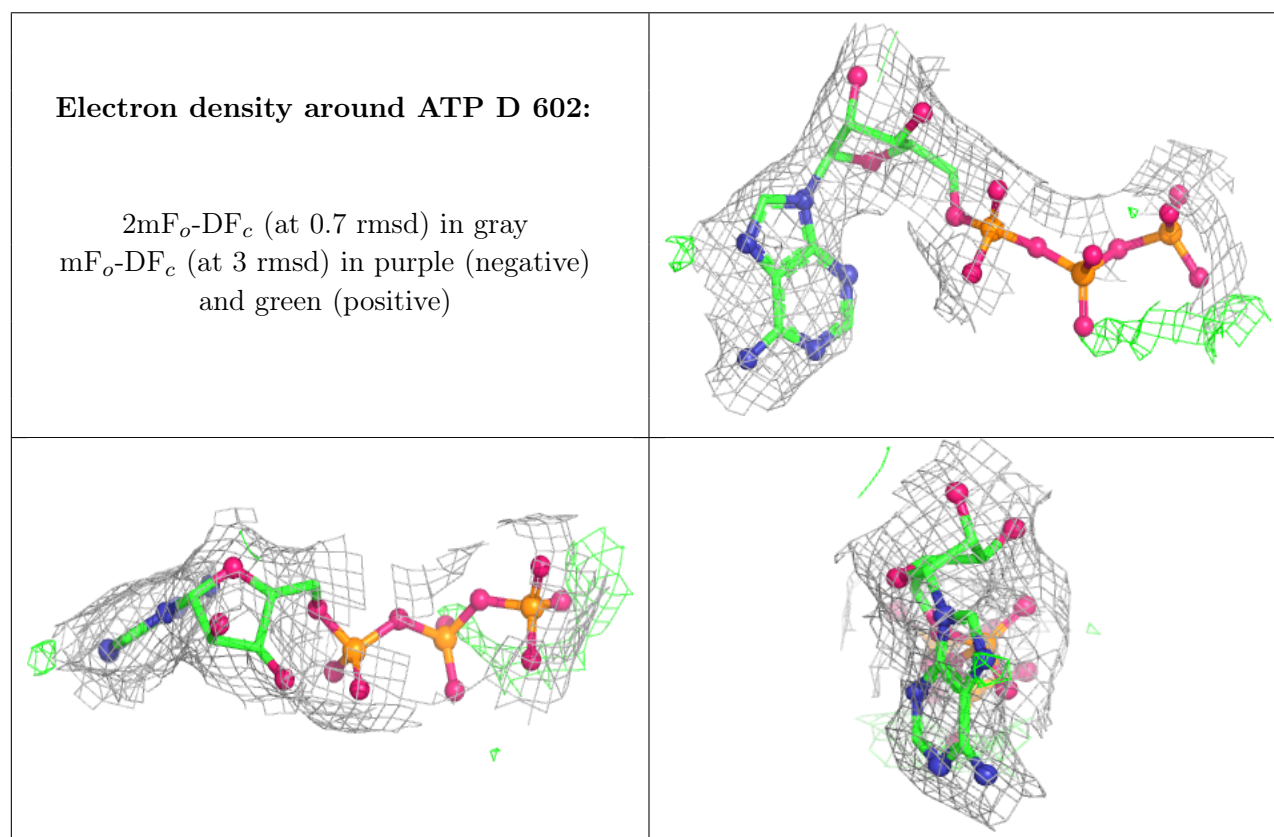
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

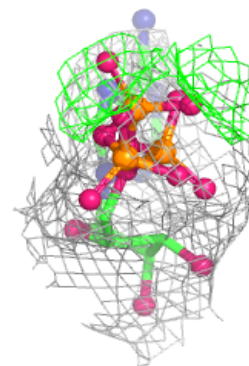
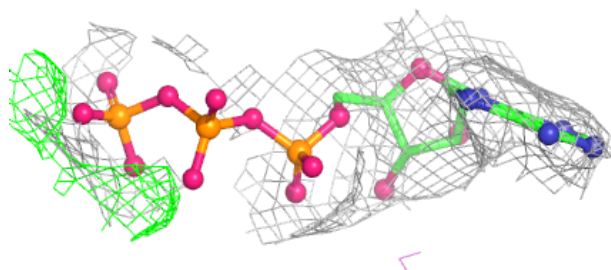
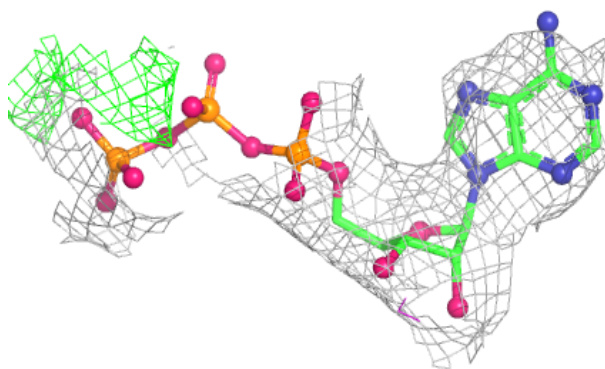
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	D	601	1/1	0.85	0.19	62,62,62,62	0
3	MG	C	601	1/1	0.86	0.20	62,62,62,62	0
3	MG	A	601	1/1	0.87	0.17	41,41,41,41	0
3	MG	B	601	1/1	0.91	0.15	51,51,51,51	0
4	ATP	D	602	31/31	0.91	0.09	55,73,87,88	0
4	ATP	C	602	31/31	0.93	0.09	58,73,92,93	0
4	ATP	B	602	31/31	0.93	0.09	53,65,76,82	0
4	ATP	A	602	31/31	0.95	0.07	53,63,80,84	0

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

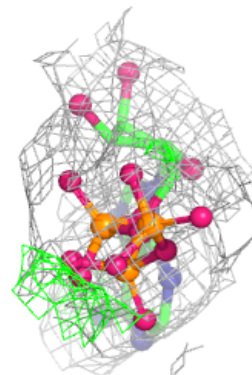
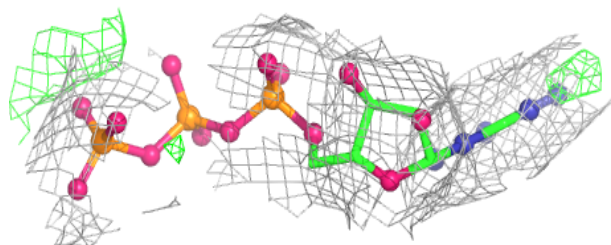
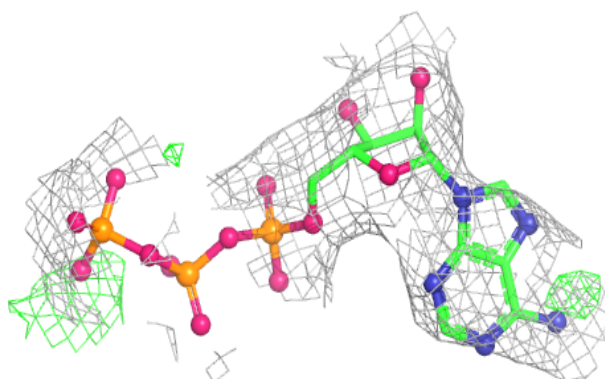


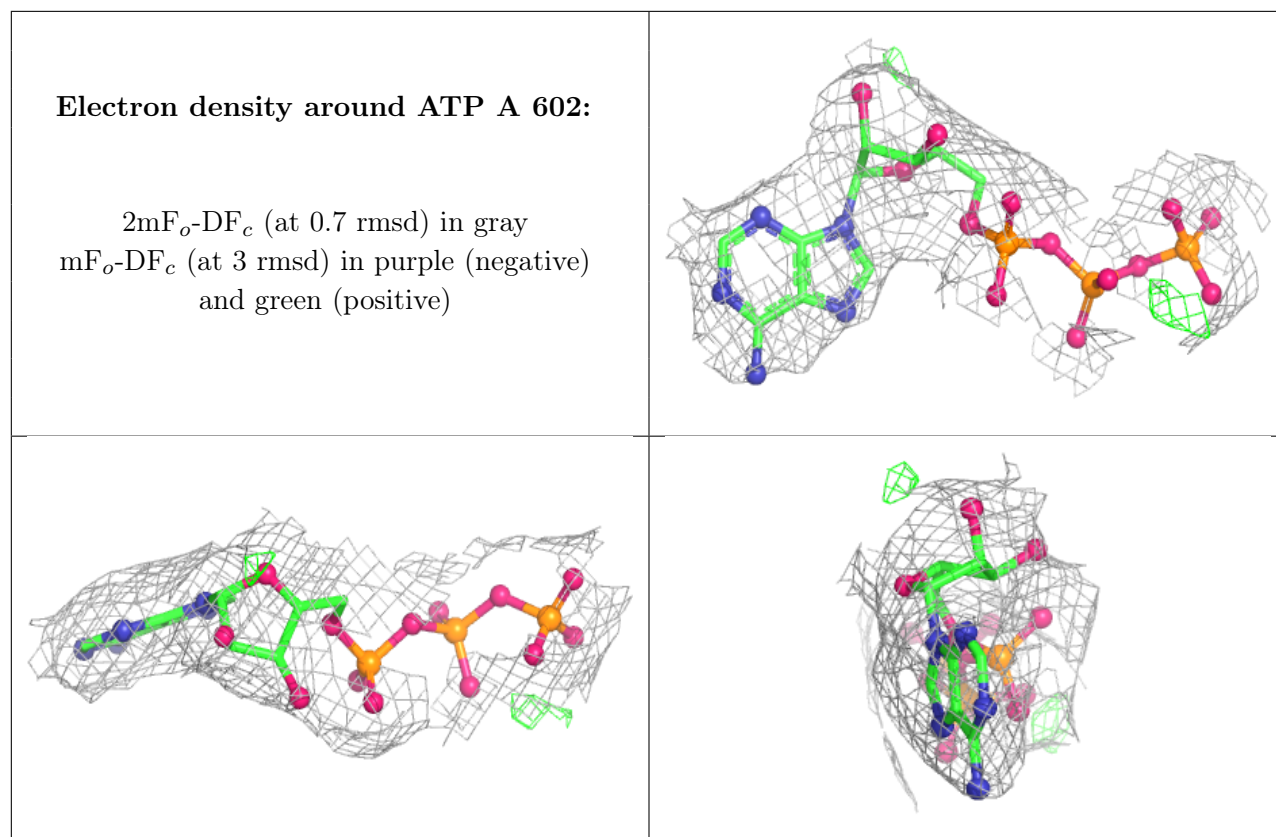
Electron density around ATP C 602:

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

**Electron density around ATP B 602:**

$2mF_o-DF_c$ (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.