



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 10:06 AM EDT

PDB ID : 6GWV
Title : Molybdenum storage protein without polymolybdate clusters and ATP
Authors : Ermler, U.; Poppe, J.; Bruenle, S.
Deposited on : 2018-06-26
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

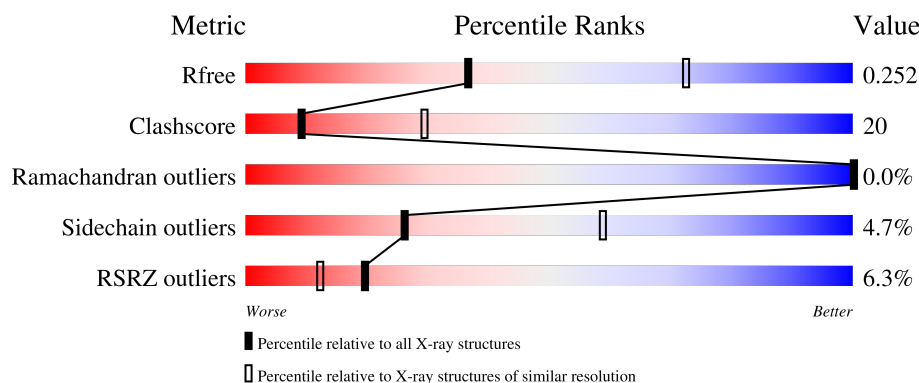
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	B	269	<div> <div>67%</div> <div>32%</div> <div>.</div> </div>
1	C	269	<div> <div>3%</div> <div>62%</div> <div>32%</div> <div>6%</div> </div>
1	E	269	<div> <div>2%</div> <div>64%</div> <div>34%</div> <div>.</div> </div>
1	H	269	<div> <div>19%</div> <div>48%</div> <div>45%</div> <div>5%</div> <div>.</div> </div>
1	I	269	<div> <div>21%</div> <div>45%</div> <div>49%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	269	
1	N	269	
1	O	269	
1	Q	269	
2	A	275	
2	D	275	
2	F	275	
2	G	275	
2	J	275	
2	L	275	
2	M	275	
2	P	275	
2	R	275	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	E	301	-	-	X	-
5	CL	M	302	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 69375 atoms, of which 35057 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 Molybdenum storage protein subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	268	Total	C	H	N	O	S	0	0	0
			4012	1255	2033	347	369	8			
1	C	268	Total	C	H	N	O	S	0	0	0
			4012	1255	2033	347	369	8			
1	E	268	Total	C	H	N	O	S	0	1	0
			4027	1260	2043	347	369	8			
1	H	268	Total	C	H	N	O	S	0	0	0
			4010	1255	2031	347	369	8			
1	I	268	Total	C	H	N	O	S	0	0	0
			4011	1255	2032	347	369	8			
1	K	268	Total	C	H	N	O	S	0	0	0
			4011	1255	2032	347	369	8			
1	N	268	Total	C	H	N	O	S	0	0	0
			4011	1255	2032	347	369	8			
1	O	268	Total	C	H	N	O	S	0	0	0
			4012	1255	2033	347	369	8			
1	Q	268	Total	C	H	N	O	S	0	0	0
			4012	1255	2033	347	369	8			

- Molecule 2 is a protein called Molybdenum storage protein subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	244	Total	C	H	N	O	S	0	0	0
			3680	1152	1859	339	327	3			
2	D	244	Total	C	H	N	O	S	0	0	0
			3680	1152	1859	339	327	3			
2	F	244	Total	C	H	N	O	S	0	0	0
			3680	1152	1859	339	327	3			
2	G	244	Total	C	H	N	O	S	0	0	0
			3680	1152	1859	339	327	3			
2	J	244	Total	C	H	N	O	S	0	0	0
			3680	1152	1859	339	327	3			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	244	Total	C	H	N	O	S	0	0	0
			3680	1152	1859	339	327	3			
2	M	244	Total	C	H	N	O	S	0	0	0
			3680	1152	1859	339	327	3			
2	P	244	Total	C	H	N	O	S	0	0	0
			3680	1152	1859	339	327	3			
2	R	244	Total	C	H	N	O	S	0	0	0
			3680	1152	1859	339	327	3			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



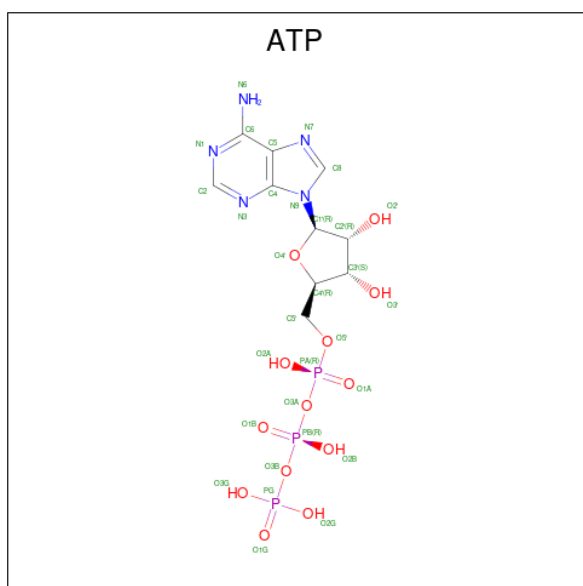
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
4	P	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

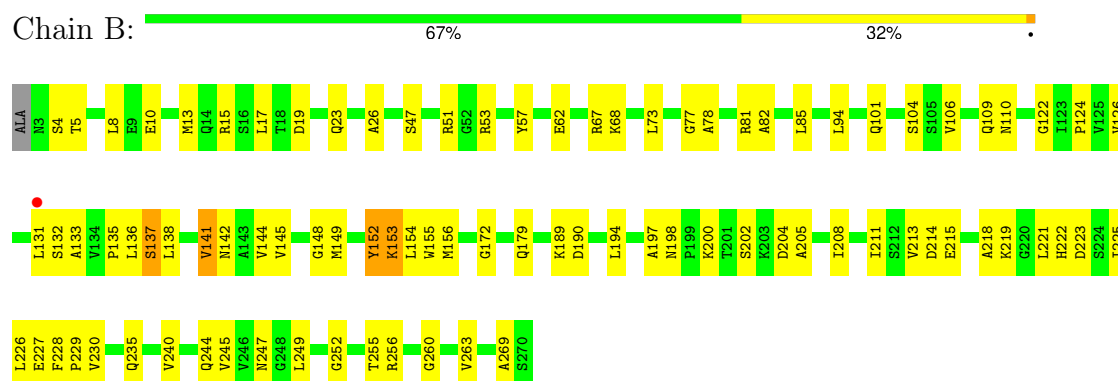
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Cl	0	0
			1	1		

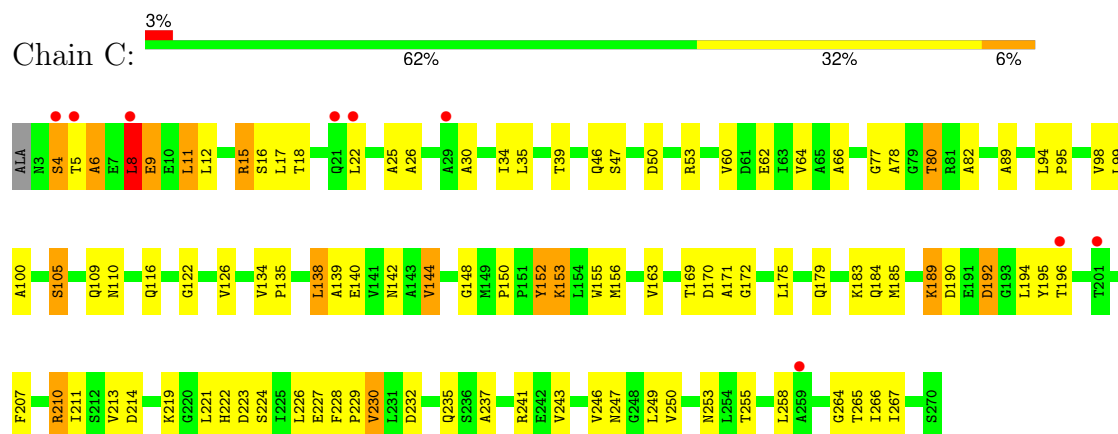
3 Residue-property plots

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

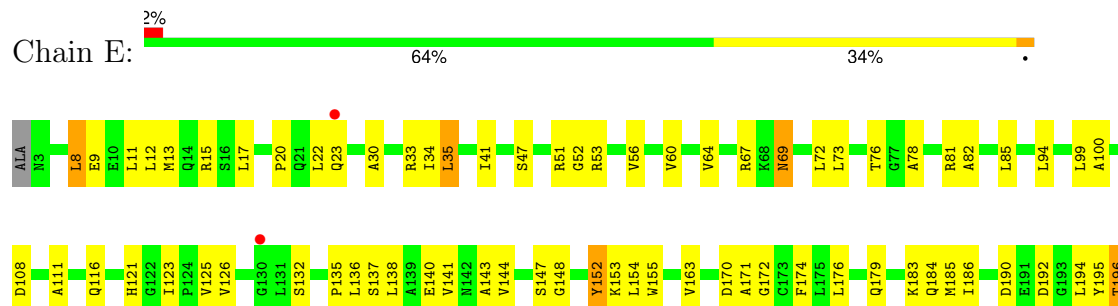
- Molecule 1: Molybdenum storage protein subunit beta



- Molecule 1: Molybdenum storage protein subunit beta

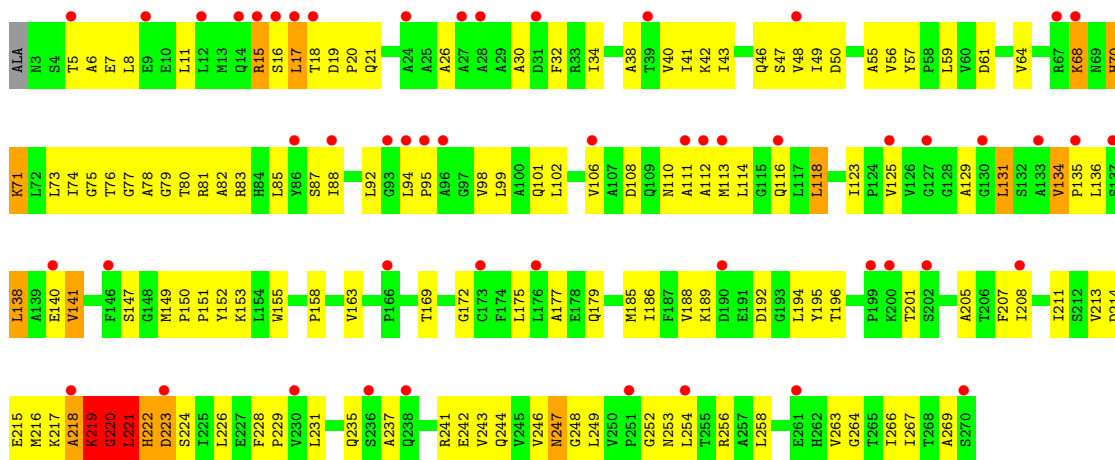


- Molecule 1: Molybdenum storage protein subunit beta

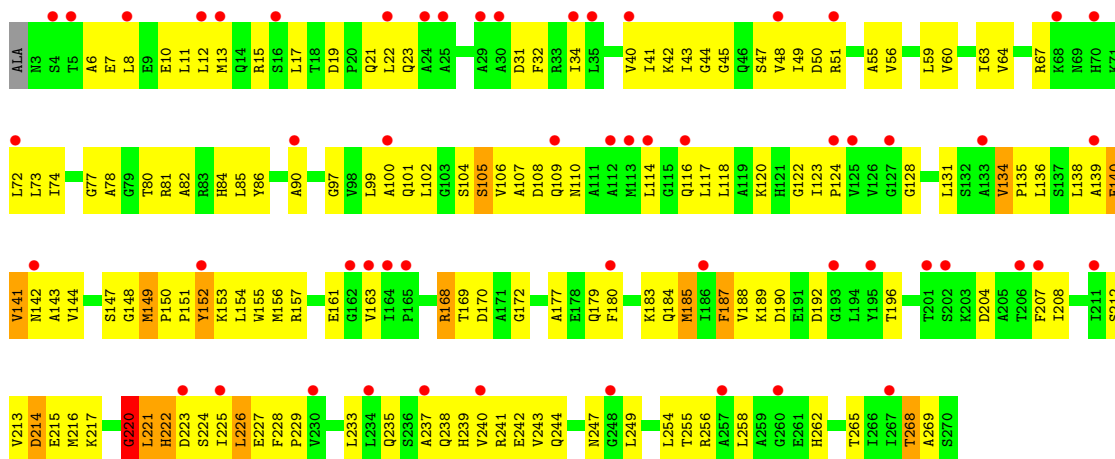
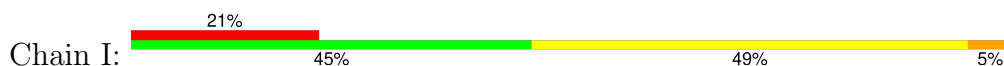




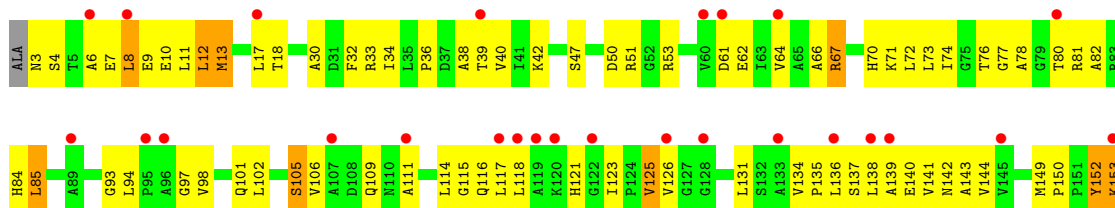
• Molecule 1: Molybdenum storage protein subunit beta

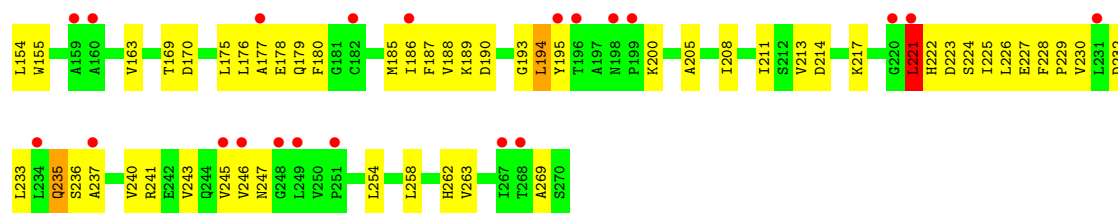


• Molecule 1: Molybdenum storage protein subunit beta

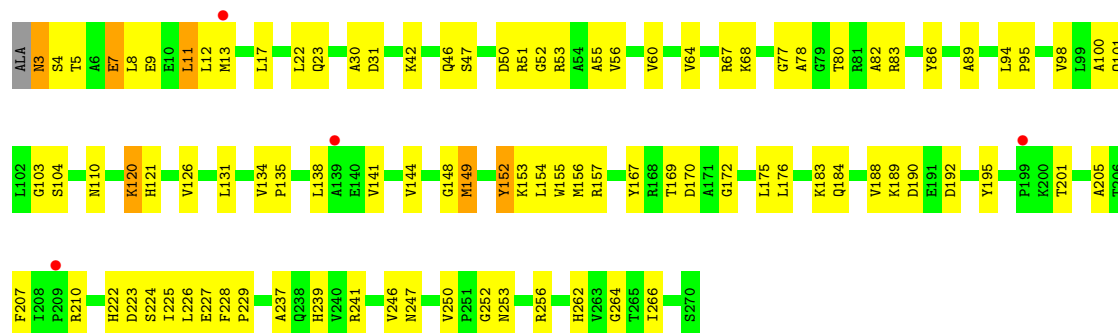


• Molecule 1: Molybdenum storage protein subunit beta

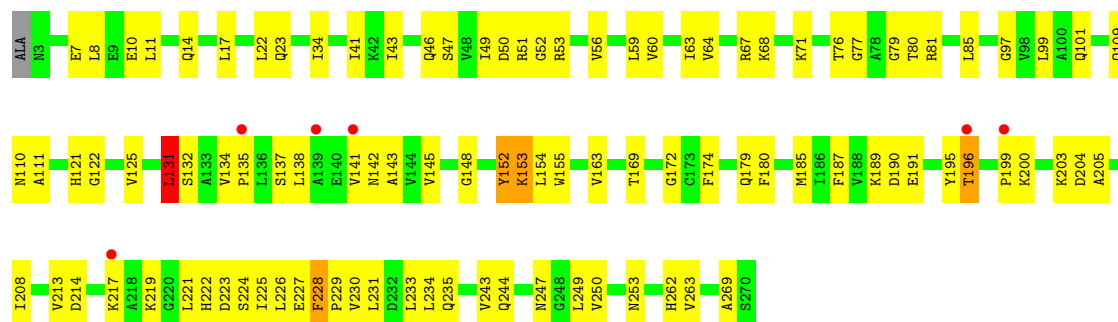




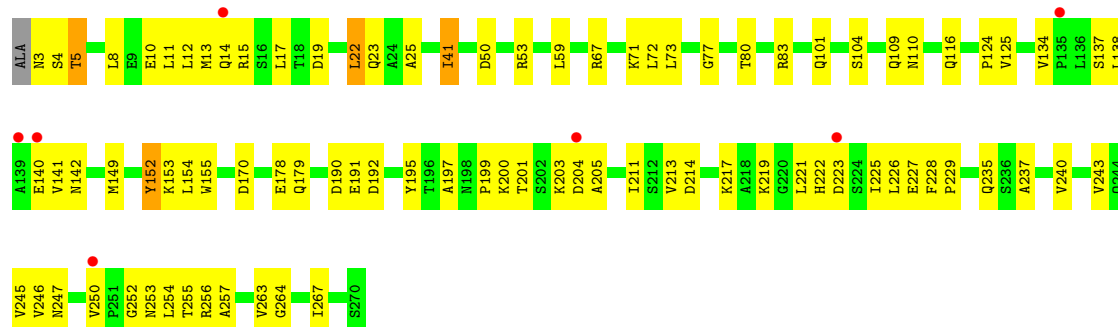
● Molecule 1: Molybdenum storage protein subunit beta



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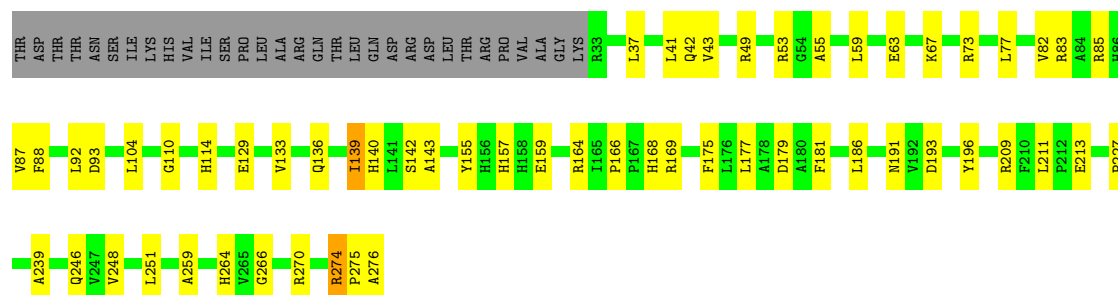


● Molecule 1: Molybdenum storage protein subunit beta



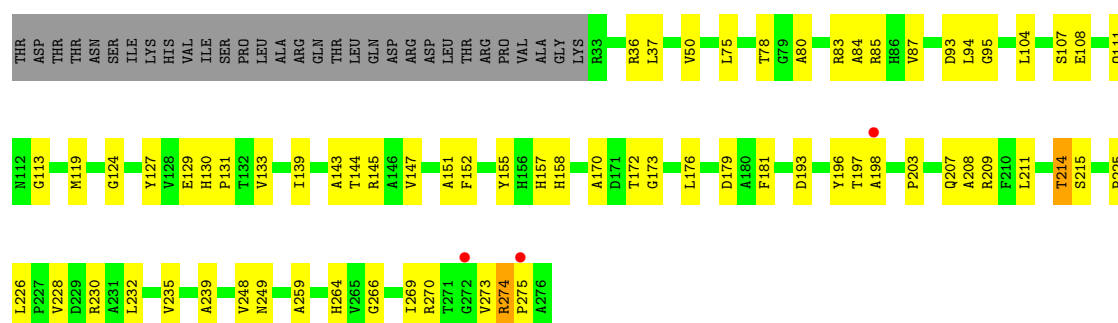
- Molecule 2: Molybdenum storage protein subunit alpha

Chain A: 



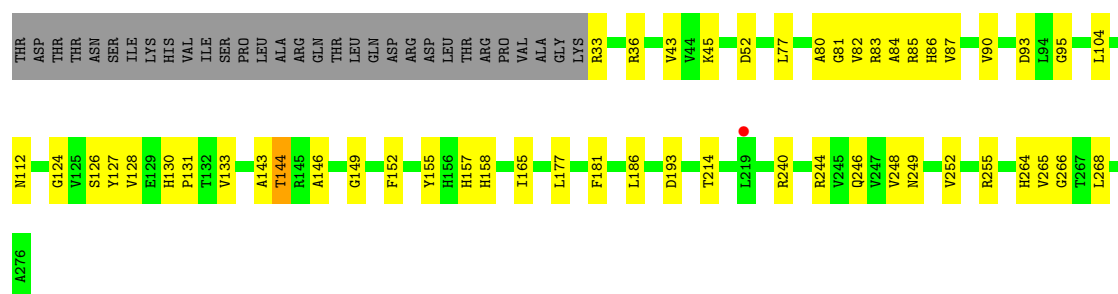
- Molecule 2: Molybdenum storage protein subunit alpha

Chain D: 



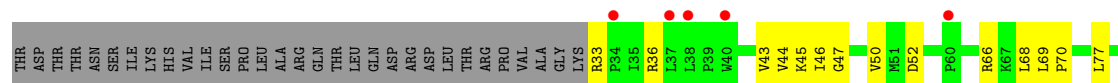
- Molecule 2: Molybdenum storage protein subunit alpha

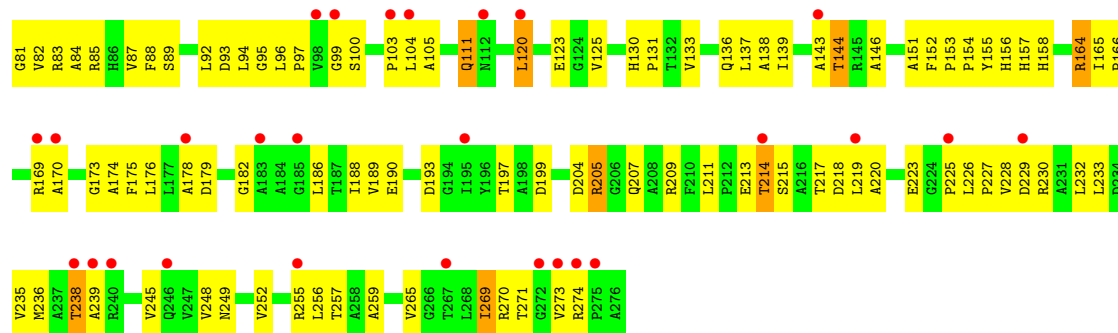
Chain F: 



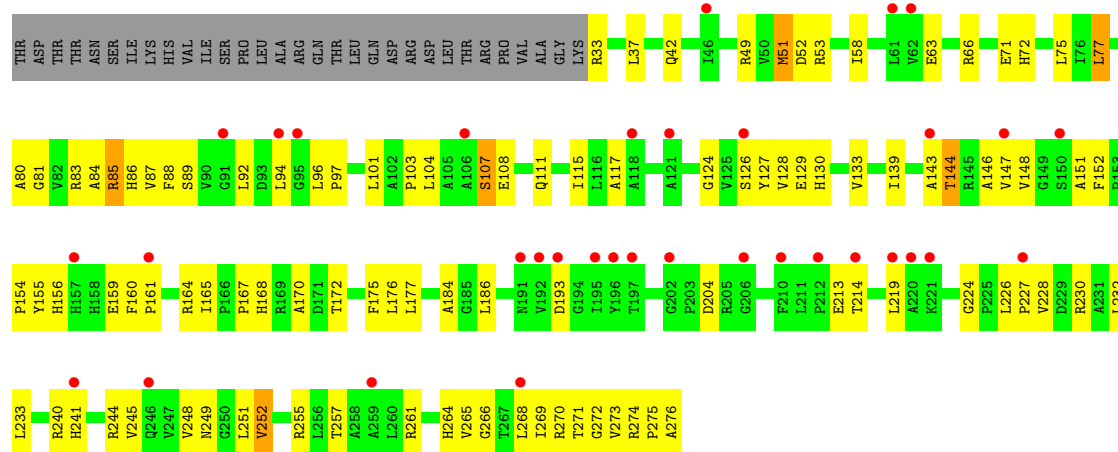
- Molecule 2: Molybdenum storage protein subunit alpha

Chain G: 

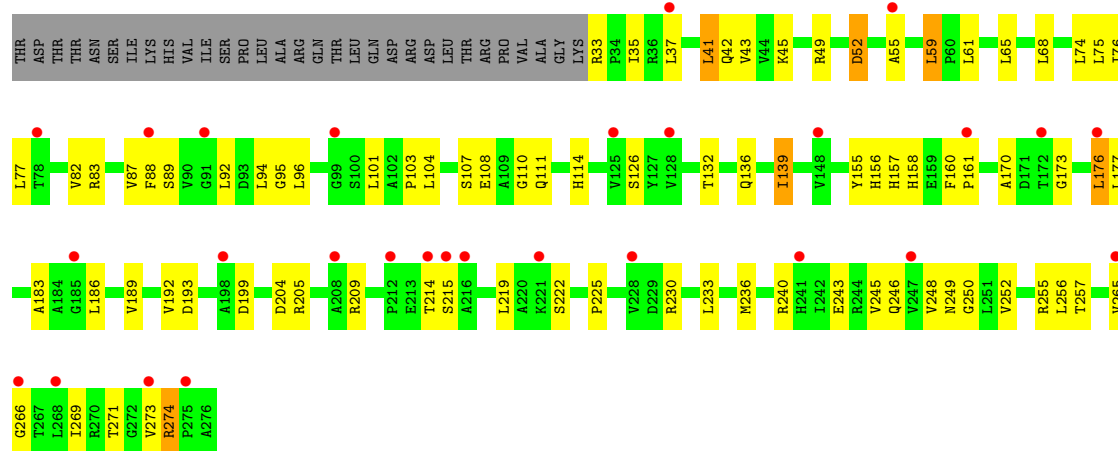




• Molecule 2: Molybdenum storage protein subunit alpha

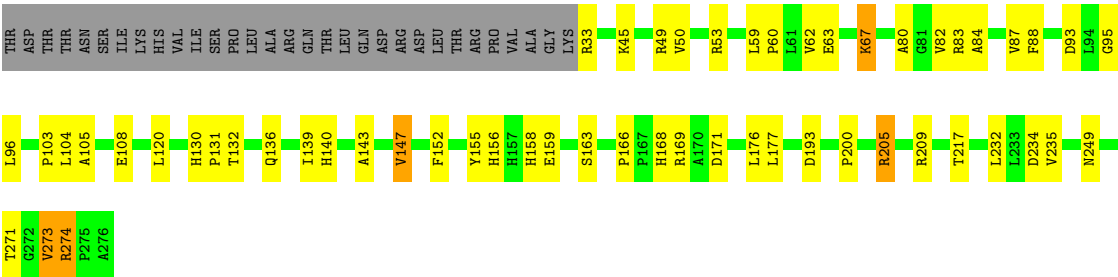


• Molecule 2: Molybdenum storage protein subunit alpha

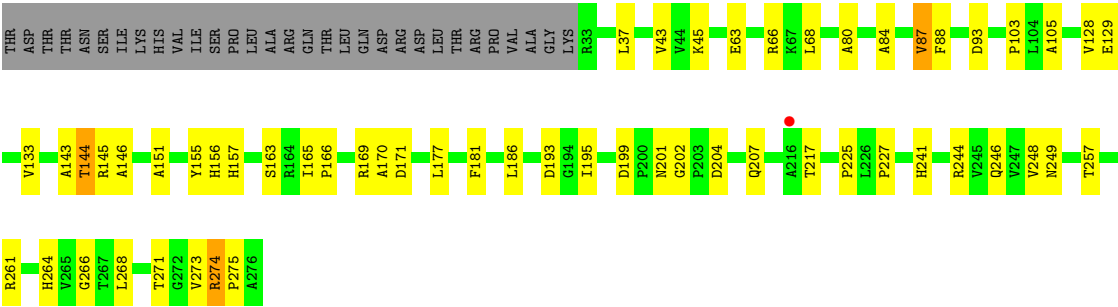


• Molecule 2: Molybdenum storage protein subunit alpha

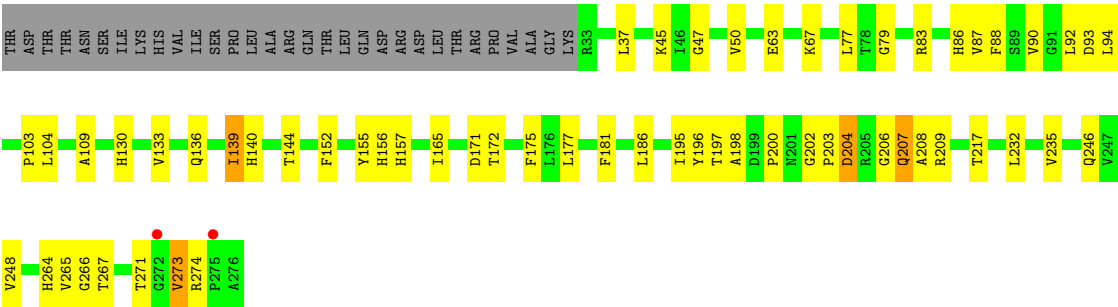




• Molecule 2: Molybdenum storage protein subunit alpha



• Molecule 2: Molybdenum storage protein subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.71Å 147.30Å 192.32Å 90.00° 107.62° 90.00°	Depositor
Resolution (Å)	47.79 – 2.80 47.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.79-2.80) 97.1 (47.79-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.233 , 0.259 0.237 , 0.252	Depositor DCC
R_{free} test set	7465 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.368 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	69375	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ATP, CL

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	B	0.34	0/2013	0.60	0/2735
1	C	0.32	0/2013	0.63	2/2735 (0.1%)
1	E	0.35	0/2021	0.61	0/2746
1	H	0.68	5/2013 (0.2%)	0.93	12/2735 (0.4%)
1	I	0.54	3/2013 (0.1%)	0.76	5/2735 (0.2%)
1	K	0.36	0/2013	0.68	1/2735 (0.0%)
1	N	0.38	0/2013	0.66	2/2735 (0.1%)
1	O	0.33	0/2013	0.62	0/2735
1	Q	0.35	0/2013	0.59	0/2735
2	A	0.29	0/1861	0.53	0/2538
2	D	0.31	0/1861	0.52	0/2538
2	F	0.29	0/1861	0.54	0/2538
2	G	0.30	0/1861	0.58	0/2538
2	J	0.29	0/1861	0.60	0/2538
2	L	0.42	1/1861 (0.1%)	0.68	3/2538 (0.1%)
2	M	0.32	0/1861	0.58	2/2538 (0.1%)
2	P	0.28	0/1861	0.50	0/2538
2	R	0.29	0/1861	0.53	0/2538
All	All	0.37	9/34874 (0.0%)	0.63	27/47468 (0.1%)

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	3
1	C	0	4
1	E	0	2
1	H	0	6
1	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	2
1	N	0	2
1	O	0	2
1	Q	0	3
2	A	0	1
2	D	0	3
2	F	0	1
2	G	0	1
2	J	0	1
2	L	0	1
2	M	0	1
2	P	0	1
2	R	0	3
All	All	0	40

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	219	LYS	CB-CG	14.47	1.91	1.52
1	H	220	GLY	CA-C	12.75	1.72	1.51
1	I	187	PHE	CE1-CZ	-11.75	1.15	1.37
1	I	187	PHE	CG-CD1	-9.89	1.24	1.38
1	H	220	GLY	N-CA	8.79	1.59	1.46
2	L	205	ARG	CD-NE	8.67	1.61	1.46
1	H	222	HIS	CA-CB	6.18	1.67	1.53
1	H	218	ALA	CA-CB	5.96	1.65	1.52
1	I	187	PHE	CD1-CE1	5.53	1.50	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	219	LYS	C-N-CA	-16.30	88.08	122.30
2	L	205	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	H	219	LYS	N-CA-C	-10.58	82.44	111.00
2	L	205	ARG	NE-CZ-NH1	9.97	125.29	120.30
2	M	205	ARG	NE-CZ-NH2	-9.33	115.63	120.30
1	I	187	PHE	CB-CG-CD2	8.78	126.94	120.80
1	H	218	ALA	N-CA-C	-8.73	87.42	111.00
1	H	218	ALA	N-CA-CB	-8.72	97.89	110.10
1	H	219	LYS	CB-CA-C	8.42	127.24	110.40
1	H	221	LEU	C-N-CA	8.22	142.24	121.70
1	K	8	LEU	CA-CB-CG	-8.06	96.77	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	218	ALA	O-C-N	-7.94	109.99	122.70
2	M	205	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	H	218	ALA	CA-C-O	-6.76	105.90	120.10
1	C	222	HIS	N-CA-CB	-6.75	98.45	110.60
1	I	221	LEU	CB-CG-CD2	6.32	121.75	111.00
1	H	219	LYS	CA-CB-CG	-5.70	100.86	113.40
1	H	222	HIS	N-CA-C	-5.66	95.73	111.00
1	H	219	LYS	CA-C-O	-5.55	108.44	120.10
1	N	11	LEU	CA-CB-CG	5.54	128.03	115.30
1	H	222	HIS	C-N-CA	5.48	135.41	121.70
1	I	220	GLY	N-CA-C	5.43	126.67	113.10
1	C	8	LEU	CA-CB-CG	-5.28	103.16	115.30
1	I	185	MET	CG-SD-CE	5.25	108.59	100.20
1	N	7	GLU	C-N-CA	5.23	134.78	121.70
1	I	221	LEU	CA-CB-CG	-5.08	103.62	115.30
2	L	205	ARG	CD-NE-CZ	-5.06	116.52	123.60

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	155	TYR	Peptide
1	B	152	TYR	Peptide
1	B	204	ASP	Peptide
1	B	4	SER	Peptide
1	C	152	TYR	Peptide
1	C	223	ASP	Peptide
1	C	6	ALA	Peptide
1	C	9	GLU	Peptide
2	D	155	TYR	Peptide
2	D	203	PRO	Peptide
2	D	274	ARG	Peptide
1	E	152	TYR	Peptide
1	E	201	THR	Peptide
2	F	155	TYR	Peptide
2	G	155	TYR	Peptide
1	H	152	TYR	Peptide
1	H	201	THR	Peptide
1	H	218	ALA	Peptide,Mainchain
1	H	219	LYS	Peptide,Mainchain
1	I	128	GLY	Peptide
1	I	152	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	I	220	GLY	Peptide
2	J	155	TYR	Peptide
1	K	152	TYR	Peptide
1	K	221	LEU	Peptide
2	L	155	TYR	Peptide
2	M	155	TYR	Peptide
1	N	152	TYR	Peptide
1	N	9	GLU	Peptide
1	O	131	LEU	Peptide
1	O	152	TYR	Peptide
2	P	155	TYR	Peptide
1	Q	152	TYR	Peptide
1	Q	4	SER	Peptide
1	Q	5	THR	Peptide
2	R	155	TYR	Peptide
2	R	204	ASP	Peptide
2	R	207	GLN	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	B	1979	2033	2032	84	2
1	C	1979	2033	2032	89	0
1	E	1984	2043	2043	82	0
1	H	1979	2031	2031	179	0
1	I	1979	2032	2032	160	0
1	K	1979	2032	2032	149	0
1	N	1979	2032	2032	89	0
1	O	1979	2033	2032	88	2
1	Q	1979	2033	2032	83	0
2	A	1821	1859	1859	45	0
2	D	1821	1859	1859	55	0
2	F	1821	1859	1859	39	0
2	G	1821	1859	1859	121	0
2	J	1821	1859	1859	95	0
2	L	1821	1859	1859	75	0
2	M	1821	1859	1859	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1821	1859	1859	41	0
2	R	1821	1859	1859	49	0
3	B	5	0	0	1	0
3	D	5	0	0	0	0
3	E	5	0	0	2	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	M	5	0	0	0	0
3	N	10	0	0	1	0
3	Q	5	0	0	0	0
3	R	5	0	0	0	0
4	A	31	12	11	3	0
4	P	31	12	12	5	0
5	M	1	0	0	2	0
All	All	34318	35057	35052	1377	2

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 20.

All (1377) 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:H:219:LYS:CG	1:H:219:LYS:CB	1.91	1.45
1:O:187:PHE:CE1	1:O:243:VAL:HG11	1.84	1.12
1:N:13:MET:O	2:M:49:ARG:NH2	1.89	1.06
2:J:224:GLY:O	2:J:230:ARG:NH2	1.89	1.05
1:H:219:LYS:CB	1:H:221:LEU:HD22	1.87	1.04
1:O:187:PHE:HE1	1:O:243:VAL:HG11	1.21	1.03
1:H:219:LYS:HB3	1:H:221:LEU:HD22	1.39	1.02
1:I:67:ARG:NH1	1:I:140:GLU:O	1.95	0.99
1:K:47:SER:O	1:K:51:ARG:NH1	1.96	0.99
1:K:40:VAL:HG11	1:K:177:ALA:HB2	1.44	0.99
2:L:252:VAL:HG21	2:L:255:ARG:HD2	1.45	0.98
1:K:221:LEU:HD22	1:K:224:SER:OG	1.64	0.98
1:I:213:VAL:O	1:I:216:MET:N	1.97	0.97
1:C:221:LEU:O	1:C:224:SER:OG	1.83	0.95
2:A:136:GLN:NE2	2:D:127:TYR:O	1.99	0.94
1:H:56:VAL:HG11	2:J:94:LEU:HD21	1.50	0.93
1:H:208:ILE:HD11	1:H:211:ILE:HG13	1.50	0.93
1:H:226:LEU:HD11	1:H:267:ILE:HD13	1.48	0.93
1:K:67:ARG:NH1	1:K:121:HIS:O	2.02	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ARG:HD2	1:B:141:VAL:O	1.69	0.92
1:H:226:LEU:HD12	1:H:231:LEU:HD21	1.51	0.92
1:H:214:ASP:O	1:H:217:LYS:HG2	1.68	0.92
2:J:83:ARG:NH1	2:J:108:GLU:OE1	2.04	0.91
1:N:262:HIS:NE2	1:N:266:ILE:HD12	1.87	0.90
1:B:67:ARG:CG	1:B:141:VAL:O	2.20	0.89
1:N:190:ASP:O	1:N:247:ASN:ND2	2.06	0.88
1:K:10:GLU:N	1:K:10:GLU:OE1	2.07	0.87
1:B:67:ARG:HG3	1:B:141:VAL:O	1.76	0.86
1:N:53:ARG:NH1	2:P:93:ASP:O	2.09	0.86
1:I:13:MET:O	2:J:49:ARG:NH2	2.09	0.86
1:O:53:ARG:NH1	2:R:93:ASP:O	2.07	0.86
1:Q:67:ARG:NH1	1:Q:140:GLU:O	2.09	0.85
1:I:213:VAL:HA	1:I:216:MET:HB2	1.57	0.85
2:J:81:GLY:O	2:J:85:ARG:NH1	2.10	0.84
1:K:227:GLU:O	1:K:230:VAL:HG12	1.77	0.84
1:O:227:GLU:O	1:O:230:VAL:HG12	1.76	0.84
1:C:8:LEU:HD13	1:C:25:ALA:HB3	1.58	0.84
1:H:219:LYS:HB3	1:H:221:LEU:CD2	2.06	0.84
1:I:225:ILE:HG23	1:I:226:LEU:HD22	1.60	0.84
1:B:260:GLY:HA3	2:M:205:ARG:HH22	1.42	0.83
1:H:216:MET:HE1	1:H:224:SER:H	1.44	0.83
2:G:136:GLN:NE2	2:J:127:TYR:O	2.11	0.82
1:E:190:ASP:O	1:E:247:ASN:ND2	2.12	0.82
1:O:190:ASP:HA	1:O:249:LEU:HD23	1.63	0.81
1:O:190:ASP:O	1:O:247:ASN:ND2	2.13	0.81
1:B:67:ARG:CD	1:B:141:VAL:O	2.28	0.81
1:H:46:GLN:OE1	1:H:83:ARG:NE	2.10	0.81
1:Q:190:ASP:O	1:Q:247:ASN:ND2	2.14	0.81
1:N:237:ALA:O	1:N:241:ARG:NH1	2.14	0.80
2:G:213:GLU:OE1	2:G:270:ARG:NH1	2.13	0.80
2:D:215:SER:HB2	2:D:270:ARG:CZ	2.12	0.80
2:G:103:PRO:HB3	2:G:156:HIS:HB3	1.63	0.80
1:Q:10:GLU:HA	1:Q:13:MET:HE2	1.63	0.80
1:I:216:MET:CE	1:I:221:LEU:HD12	2.12	0.80
1:B:213:VAL:HG21	1:B:235:GLN:CG	2.13	0.79
2:A:213:GLU:OE2	2:A:270:ARG:NH1	2.15	0.79
1:H:219:LYS:HD2	1:H:220:GLY:H	1.47	0.79
2:R:87:VAL:HG11	2:R:104:LEU:HB3	1.64	0.79
1:H:219:LYS:HB2	1:H:221:LEU:HD22	1.64	0.79
1:H:11:LEU:O	1:H:15:ARG:HB2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ARG:NH1	2:F:93:ASP:O	2.16	0.79
2:G:81:GLY:O	2:G:85:ARG:NH1	2.16	0.79
1:I:242:GLU:O	1:I:243:VAL:HG23	1.82	0.78
1:O:187:PHE:CD1	1:O:243:VAL:HG11	2.19	0.78
1:H:226:LEU:HD11	1:H:267:ILE:CD1	2.14	0.78
1:H:101:GLN:HG3	1:H:153:LYS:HB3	1.66	0.77
1:K:241:ARG:HE	1:K:269:ALA:HB3	1.48	0.77
1:H:108:ASP:OD1	1:H:147:SER:OG	2.01	0.77
1:I:216:MET:HE3	1:I:221:LEU:HD12	1.67	0.77
1:E:69:ASN:O	1:E:69:ASN:ND2	2.17	0.77
2:A:139:ILE:HD11	2:D:147:VAL:HG12	1.66	0.77
1:C:190:ASP:O	1:C:247:ASN:ND2	2.18	0.77
1:H:101:GLN:CG	1:H:153:LYS:HB3	2.15	0.77
2:G:36:ARG:NH1	2:G:182:GLY:O	2.18	0.76
1:B:47:SER:O	1:B:51:ARG:NE	2.18	0.76
1:H:219:LYS:CG	1:H:219:LYS:CA	2.64	0.75
1:C:8:LEU:CD1	1:C:25:ALA:HB3	2.16	0.75
1:I:216:MET:HE3	1:I:221:LEU:CD1	2.16	0.75
2:M:33:ARG:NH1	2:M:274:ARG:O	2.19	0.75
1:I:212:SER:O	1:I:215:GLU:HB2	1.86	0.75
1:I:10:GLU:N	1:I:10:GLU:OE1	2.19	0.74
1:O:244:GLN:NE2	1:O:263:VAL:O	2.20	0.74
2:J:33:ARG:HE	2:J:241:HIS:CD2	2.04	0.74
2:J:193:ASP:HA	2:J:249:ASN:HB2	1.67	0.74
1:H:151:PRO:HD3	2:G:158:HIS:CD2	2.22	0.74
1:B:189:LYS:NZ	1:B:225:ILE:O	2.20	0.74
2:M:93:ASP:O	1:Q:53:ARG:NH1	2.20	0.74
1:H:7:GLU:HG2	1:H:11:LEU:HD13	1.69	0.73
1:B:190:ASP:O	1:B:247:ASN:ND2	2.22	0.73
1:Q:101:GLN:HB3	1:Q:153:LYS:HD3	1.70	0.73
1:K:8:LEU:O	1:K:11:LEU:N	2.21	0.73
2:P:45:LYS:NZ	2:P:171:ASP:OD1	2.20	0.73
1:N:7:GLU:OE2	1:N:11:LEU:HD12	1.89	0.73
1:O:71:LYS:NZ	1:O:142:ASN:OD1	2.22	0.72
1:B:213:VAL:HG21	1:B:235:GLN:HG2	1.71	0.72
1:I:118:LEU:HB3	1:I:123:ILE:CG2	2.20	0.72
2:J:228:VAL:HB	2:J:232:LEU:HD23	1.71	0.72
2:D:87:VAL:HG11	2:D:104:LEU:HB3	1.71	0.72
1:K:8:LEU:O	1:K:12:LEU:N	2.20	0.72
1:K:190:ASP:O	1:K:247:ASN:ND2	2.23	0.71
1:Q:101:GLN:CB	1:Q:153:LYS:HD3	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:262:HIS:O	1:N:262:HIS:ND1	2.23	0.71
1:I:15:ARG:NH1	1:I:19:ASP:OD2	2.23	0.71
1:H:219:LYS:HD2	1:H:220:GLY:N	2.05	0.71
1:N:223:ASP:HB2	1:N:228:PHE:HB3	1.73	0.70
1:Q:8:LEU:HD21	1:Q:25:ALA:HB1	1.72	0.70
1:H:134:VAL:HG12	1:H:135:PRO:HD3	1.73	0.70
1:K:154:LEU:HD22	2:L:177:LEU:HD12	1.72	0.70
1:Q:225:ILE:HG23	1:Q:226:LEU:CD1	2.21	0.70
1:I:81:ARG:NE	2:L:87:VAL:HG22	2.07	0.70
2:G:138:ALA:HB1	2:J:124:GLY:HA2	1.74	0.70
1:B:77:GLY:O	1:B:110:ASN:ND2	2.23	0.70
1:C:8:LEU:HD21	1:C:22:LEU:O	1.92	0.70
1:H:85:LEU:HD21	2:J:83:ARG:NH1	2.07	0.69
1:C:138:LEU:HD23	1:E:138:LEU:HD21	1.74	0.69
1:B:57:TYR:OH	2:D:94:LEU:O	2.10	0.69
1:E:225:ILE:HG23	1:E:226:LEU:HG	1.75	0.69
1:B:53:ARG:NH1	2:D:93:ASP:O	2.26	0.69
1:N:253:ASN:OD1	1:N:256:ARG:NH2	2.26	0.69
2:G:45:LYS:HE3	2:G:170:ALA:HB1	1.74	0.69
1:I:12:LEU:HD13	2:J:89:SER:HB3	1.74	0.69
1:I:42:LYS:N	1:I:185:MET:HE1	2.08	0.69
2:L:252:VAL:HG23	2:L:252:VAL:O	1.94	0.68
1:H:219:LYS:HB3	1:H:221:LEU:HD13	1.76	0.68
1:I:190:ASP:HA	1:I:249:LEU:HD23	1.74	0.68
1:I:17:LEU:HD12	1:I:17:LEU:H	1.58	0.68
1:N:11:LEU:O	1:N:11:LEU:HD23	1.94	0.68
2:M:87:VAL:HG11	2:M:104:LEU:HB3	1.75	0.68
1:H:113:MET:HG3	2:J:104:LEU:HD11	1.75	0.68
1:N:17:LEU:O	1:N:23:GLN:NE2	2.25	0.68
2:M:200:PRO:O	2:M:205:ARG:HD3	1.93	0.68
2:M:147:VAL:HG13	2:R:139:ILE:HD11	1.74	0.68
2:D:129:GLU:O	2:D:133:VAL:HG23	1.94	0.68
1:K:13:MET:SD	1:K:13:MET:N	2.66	0.68
2:D:239:ALA:O	2:D:273:VAL:HG21	1.94	0.67
2:P:63:GLU:OE2	2:P:66:ARG:NH2	2.24	0.67
1:Q:225:ILE:HG23	1:Q:226:LEU:HD12	1.74	0.67
1:Q:8:LEU:O	1:Q:11:LEU:N	2.27	0.67
2:J:87:VAL:HG11	2:J:104:LEU:HB3	1.75	0.67
1:K:8:LEU:N	1:K:8:LEU:HD12	2.09	0.67
1:E:211:ILE:HD13	1:E:216:MET:HG2	1.76	0.67
1:O:247:ASN:OD1	1:O:250:VAL:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:264:HIS:NE2	2:F:266:GLY:O	2.27	0.67
1:H:34:ILE:HG23	1:K:116:GLN:O	1.95	0.67
1:I:77:GLY:HA2	1:I:169:THR:HG21	1.76	0.67
1:I:86:TYR:O	1:I:90:ALA:HB3	1.94	0.67
1:H:56:VAL:CG1	2:J:94:LEU:HD21	2.25	0.66
1:Q:10:GLU:HA	1:Q:13:MET:CE	2.25	0.66
1:I:185:MET:HB3	1:I:243:VAL:HG21	1.75	0.66
1:H:94:LEU:HB3	1:H:98:VAL:HG21	1.78	0.66
1:I:40:VAL:HG13	1:I:185:MET:SD	2.35	0.66
2:D:144:THR:HG22	2:D:145:ARG:H	1.61	0.66
2:F:193:ASP:HA	2:F:249:ASN:HB2	1.76	0.66
1:K:38:ALA:HA	1:K:71:LYS:HB2	1.77	0.66
1:K:135:PRO:O	1:K:141:VAL:HG13	1.95	0.66
1:K:222:HIS:HB3	1:K:228:PHE:CD1	2.31	0.66
1:B:194:LEU:HD11	1:B:221:LEU:HD12	1.78	0.65
2:J:128:VAL:HG23	2:J:133:VAL:HG12	1.78	0.65
2:R:47:GLY:O	2:R:50:VAL:HG22	1.97	0.65
1:B:260:GLY:HA3	2:M:205:ARG:NH2	2.11	0.65
1:H:185:MET:HB3	1:H:243:VAL:HG13	1.76	0.65
1:K:9:GLU:HG3	2:L:89:SER:OG	1.96	0.65
2:J:77:LEU:HD21	2:J:177:LEU:HD23	1.77	0.65
2:P:129:GLU:O	2:P:133:VAL:HG23	1.96	0.65
1:H:219:LYS:CB	1:H:221:LEU:CD2	2.68	0.65
1:K:138:LEU:HB3	1:K:140:GLU:CD	2.17	0.65
1:B:47:SER:OG	3:B:301:SO4:O4	2.13	0.65
2:G:214:THR:HG21	2:G:219:LEU:HD21	1.79	0.65
1:I:104:SER:HA	1:I:149:MET:HG2	1.77	0.65
1:N:8:LEU:CD2	1:N:12:LEU:HG	2.26	0.65
2:P:80:ALA:N	4:P:301:ATP:O2G	2.29	0.65
2:J:214:THR:HG21	2:J:219:LEU:HD21	1.78	0.65
1:O:243:VAL:HG12	1:O:244:GLN:N	2.11	0.65
1:H:7:GLU:CG	1:H:11:LEU:HD13	2.27	0.65
1:K:3:ASN:ND2	1:K:7:GLU:OE1	2.27	0.65
1:N:252:GLY:O	1:N:256:ARG:HG3	1.97	0.65
1:I:244:GLN:HG3	1:I:265:THR:O	1.96	0.64
2:J:168:HIS:HA	2:J:172:THR:HG21	1.78	0.64
1:B:213:VAL:HG21	1:B:235:GLN:CD	2.18	0.64
1:K:179:GLN:HG3	2:L:157:HIS:O	1.97	0.64
2:P:103:PRO:HB3	2:P:156:HIS:HB3	1.79	0.64
2:L:83:ARG:NE	2:L:108:GLU:OE1	2.29	0.64
1:E:17:LEU:HD11	2:F:85:ARG:NE	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:52:ASP:OD2	2:L:82:VAL:HG12	1.97	0.64
1:Q:134:VAL:O	1:Q:138:LEU:HD13	1.97	0.64
1:B:154:LEU:HD23	2:A:177:LEU:HD11	1.80	0.64
1:C:78:ALA:HB1	1:C:82:ALA:HB2	1.78	0.64
1:Q:203:LYS:HG3	1:Q:204:ASP:N	2.12	0.64
1:H:213:VAL:HG21	1:H:235:GLN:CG	2.27	0.64
1:I:213:VAL:HA	1:I:216:MET:CB	2.27	0.64
2:J:172:THR:HA	2:J:232:LEU:HD13	1.80	0.64
2:G:189:VAL:HG22	2:G:256:LEU:HD13	1.80	0.64
1:Q:252:GLY:O	1:Q:256:ARG:HG3	1.97	0.63
1:H:15:ARG:NH1	1:H:19:ASP:OD2	2.31	0.63
1:I:118:LEU:HB3	1:I:123:ILE:HG22	1.78	0.63
1:I:154:LEU:HD23	2:J:177:LEU:HD12	1.81	0.63
1:H:219:LYS:CG	1:H:219:LYS:HA	2.28	0.63
1:H:221:LEU:C	1:H:223:ASP:H	1.88	0.63
1:O:190:ASP:HA	1:O:249:LEU:CD2	2.27	0.63
1:I:97:GLY:O	1:I:153:LYS:O	2.15	0.63
1:K:178:GLU:OE2	1:K:237:ALA:HB1	1.99	0.63
1:H:223:ASP:OD1	1:H:228:PHE:HB3	1.97	0.63
1:K:6:ALA:O	1:K:10:GLU:OE1	2.15	0.63
1:H:214:ASP:HA	1:H:217:LYS:HE2	1.79	0.63
1:H:219:LYS:HB3	1:H:221:LEU:CD1	2.28	0.63
1:H:221:LEU:HD13	1:H:221:LEU:N	2.14	0.63
1:N:262:HIS:CE1	1:N:266:ILE:HG13	2.33	0.63
1:N:8:LEU:HD23	1:N:12:LEU:HG	1.81	0.63
2:R:198:ALA:HB3	2:R:208:ALA:HB2	1.81	0.62
2:G:152:PHE:CE1	2:G:170:ALA:HB2	2.34	0.62
1:O:262:HIS:O	1:O:262:HIS:ND1	2.32	0.62
1:C:192:ASP:HA	1:C:247:ASN:HB2	1.80	0.62
1:H:213:VAL:HG21	1:H:235:GLN:HG2	1.81	0.62
1:I:235:GLN:NE2	1:I:269:ALA:O	2.33	0.62
1:Q:77:GLY:O	1:Q:110:ASN:ND2	2.22	0.62
1:K:7:GLU:O	1:K:10:GLU:HB2	2.00	0.62
2:A:63:GLU:O	2:A:67:LYS:HG2	1.98	0.62
1:C:8:LEU:HD13	1:C:25:ALA:CB	2.28	0.62
1:K:221:LEU:HD22	1:K:224:SER:HG	1.63	0.62
1:B:17:LEU:O	1:B:23:GLN:NE2	2.29	0.62
1:K:237:ALA:HA	2:L:161:PRO:HB2	1.82	0.62
1:N:195:TYR:HB3	1:N:205:ALA:HB1	1.82	0.61
2:P:264:HIS:NE2	2:P:266:GLY:O	2.34	0.61
1:H:208:ILE:CD1	1:H:211:ILE:HG13	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:109:GLN:NE2	2:R:104:LEU:O	2.32	0.61
1:B:197:ALA:HB3	1:B:202:SER:HB2	1.81	0.61
2:M:45:LYS:NZ	2:M:171:ASP:OD1	2.27	0.61
1:C:152:TYR:OH	2:D:158:HIS:O	2.17	0.61
1:C:170:ASP:OD1	1:C:189:LYS:NZ	2.33	0.61
1:I:74:ILE:HD12	1:I:123:ILE:HD11	1.83	0.61
2:J:128:VAL:HG23	2:J:133:VAL:CG1	2.30	0.61
1:N:101:GLN:HB3	1:N:153:LYS:HB3	1.82	0.61
1:Q:101:GLN:HB3	1:Q:153:LYS:HB3	1.83	0.61
1:N:42:LYS:NZ	1:N:170:ASP:OD1	2.30	0.61
1:Q:246:VAL:HG13	1:Q:253:ASN:HB3	1.82	0.61
1:C:183:LYS:HG3	1:C:184:GLN:HG3	1.82	0.61
1:I:60:VAL:O	1:I:64:VAL:HG23	2.00	0.61
1:N:188:VAL:HG12	1:N:246:VAL:CG2	2.30	0.61
1:N:262:HIS:NE2	1:N:266:ILE:CD1	2.63	0.61
1:I:220:GLY:O	1:I:222:HIS:N	2.34	0.61
1:Q:223:ASP:HB2	1:Q:228:PHE:HB3	1.81	0.61
1:H:43:ILE:HB	1:H:49:ILE:HD11	1.83	0.61
2:G:214:THR:CG2	2:G:219:LEU:HD11	2.31	0.60
1:I:184:GLN:NE2	1:I:258:LEU:O	2.30	0.60
1:O:131:LEU:HB2	1:O:180:PHE:HZ	1.64	0.60
1:E:47:SER:O	1:E:51:ARG:NE	2.33	0.60
1:I:59:LEU:HD23	1:I:254:LEU:HD12	1.84	0.60
2:R:202:GLY:O	2:R:204:ASP:N	2.33	0.60
1:H:40:VAL:HG22	1:H:73:LEU:HB2	1.83	0.60
2:G:186:LEU:O	2:G:245:VAL:HG13	2.02	0.60
1:K:175:LEU:HD21	1:K:233:LEU:HD13	1.83	0.60
1:H:138:LEU:HD11	1:K:138:LEU:HD21	1.84	0.60
1:I:138:LEU:HD13	1:K:138:LEU:HD11	1.82	0.60
2:J:275:PRO:O	2:J:276:ALA:HB2	2.02	0.60
1:O:76:THR:HG21	1:O:111:ALA:HA	1.84	0.60
2:R:45:LYS:NZ	2:R:171:ASP:OD1	2.27	0.60
2:J:193:ASP:OD1	2:J:249:ASN:ND2	2.34	0.60
1:K:134:VAL:O	1:K:138:LEU:HD13	2.02	0.60
2:L:87:VAL:HG11	2:L:104:LEU:HB3	1.82	0.60
1:Q:134:VAL:O	1:Q:138:LEU:CD1	2.50	0.60
1:C:190:ASP:HA	1:C:249:LEU:HD23	1.83	0.60
1:E:196:THR:HA	1:E:221:LEU:HD11	1.83	0.60
1:N:138:LEU:CD2	1:Q:138:LEU:HD21	2.32	0.60
1:H:211:ILE:HG23	1:H:215:GLU:HB2	1.84	0.59
2:J:80:ALA:HB1	2:J:84:ALA:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:LEU:O	1:E:11:LEU:N	2.35	0.59
1:I:55:ALA:O	1:I:59:LEU:HD12	2.02	0.59
1:N:95:PRO:HG2	1:N:98:VAL:HG23	1.83	0.59
1:Q:71:LYS:NZ	1:Q:142:ASN:OD1	2.35	0.59
1:E:34:ILE:HG22	1:E:35:LEU:HD13	1.84	0.59
1:H:112:ALA:O	1:H:116:GLN:HG3	2.02	0.59
1:N:77:GLY:O	1:N:110:ASN:ND2	2.31	0.59
2:A:37:LEU:N	2:A:181:PHE:O	2.35	0.59
1:E:47:SER:N	3:E:301:SO4:O2	2.35	0.59
1:E:67:ARG:HD2	1:E:141:VAL:O	2.03	0.59
1:H:18:THR:OG1	2:G:225:PRO:HA	2.03	0.59
1:N:8:LEU:HG	1:N:11:LEU:HB3	1.84	0.59
4:P:301:ATP:N3	4:P:301:ATP:H2'	2.17	0.59
1:E:94:LEU:O	1:E:163:VAL:HG11	2.03	0.59
1:H:216:MET:HE1	1:H:224:SER:N	2.14	0.59
2:G:94:LEU:HD23	1:K:53:ARG:HB2	1.85	0.59
2:P:204:ASP:O	2:P:207:GLN:N	2.36	0.59
1:N:67:ARG:HE	1:N:68:LYS:HZ1	1.50	0.59
1:I:77:GLY:O	1:I:110:ASN:ND2	2.30	0.59
1:O:243:VAL:CG1	1:O:244:GLN:N	2.65	0.59
1:C:243:VAL:O	1:C:266:ILE:HG23	2.03	0.59
1:H:50:ASP:OD2	1:H:80:THR:HG22	2.03	0.59
1:K:76:THR:HG21	1:K:111:ALA:HA	1.85	0.58
2:J:241:HIS:C	2:J:273:VAL:HG11	2.23	0.58
2:R:88:PHE:O	2:R:92:LEU:N	2.31	0.58
1:K:213:VAL:HG21	1:K:235:GLN:HG2	1.84	0.58
1:N:3:ASN:N	1:N:3:ASN:OD1	2.36	0.58
1:B:219:LYS:CB	1:B:221:LEU:HD23	2.34	0.58
1:I:138:LEU:O	1:I:142:ASN:N	2.36	0.58
1:I:149:MET:SD	1:I:169:THR:HG22	2.43	0.58
1:N:60:VAL:O	1:N:64:VAL:HG23	2.03	0.58
1:O:7:GLU:O	1:O:11:LEU:N	2.36	0.58
1:H:226:LEU:CD1	1:H:231:LEU:HD21	2.30	0.58
2:P:244:ARG:HD2	2:P:268:LEU:HD22	1.85	0.58
1:K:6:ALA:HB2	1:N:3:ASN:N	2.18	0.58
1:B:94:LEU:HD21	2:D:119:MET:SD	2.44	0.58
2:J:264:HIS:NE2	2:J:266:GLY:O	2.36	0.58
1:Q:41:ILE:HD11	1:Q:72:LEU:HD22	1.86	0.58
2:L:103:PRO:HB3	2:L:156:HIS:HB3	1.85	0.58
2:J:88:PHE:O	2:J:92:LEU:N	2.23	0.57
1:K:51:ARG:HH12	1:K:190:ASP:HB3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:136:GLN:O	2:L:139:ILE:HG23	2.04	0.57
1:C:190:ASP:HA	1:C:249:LEU:CD2	2.34	0.57
1:I:107:ALA:HB1	1:I:147:SER:O	2.03	0.57
1:O:101:GLN:HB3	1:O:153:LYS:HB3	1.86	0.57
1:E:171:ALA:HB2	1:E:230:VAL:CG2	2.35	0.57
1:H:217:LYS:HA	1:H:222:HIS:HA	1.87	0.57
1:B:131:LEU:HD13	1:E:125:VAL:HG21	1.86	0.57
2:G:151:ALA:HB1	2:G:174:ALA:HB2	1.87	0.57
1:I:240:VAL:HG13	1:I:241:ARG:H	1.70	0.57
1:H:216:MET:CE	1:H:224:SER:H	2.16	0.57
1:I:42:LYS:NZ	1:I:170:ASP:OD1	2.27	0.57
1:K:225:ILE:HG23	1:K:226:LEU:HD12	1.85	0.57
1:C:62:GLU:OE1	1:C:255:THR:OG1	2.22	0.57
1:H:246:VAL:HG13	1:H:253:ASN:HB3	1.86	0.57
2:G:103:PRO:HB3	2:G:156:HIS:CB	2.33	0.57
1:I:15:ARG:NH1	1:I:21:GLN:OE1	2.35	0.57
2:P:199:ASP:HB2	2:P:225:PRO:HG2	1.86	0.57
1:B:152:TYR:O	1:B:155:TRP:N	2.37	0.57
1:I:40:VAL:CG1	1:I:177:ALA:HB2	2.35	0.57
1:K:47:SER:OG	1:K:189:LYS:HG2	2.05	0.57
1:C:221:LEU:HB3	1:C:224:SER:OG	2.04	0.56
1:I:152:TYR:O	1:I:155:TRP:N	2.37	0.56
2:J:53:ARG:NE	2:J:53:ARG:HA	2.19	0.56
1:O:179:GLN:HG3	2:P:157:HIS:O	2.04	0.56
1:B:138:LEU:HB2	1:B:141:VAL:CG2	2.35	0.56
1:B:154:LEU:HD23	2:A:177:LEU:CD1	2.35	0.56
2:A:275:PRO:O	2:A:276:ALA:HB2	2.05	0.56
1:C:12:LEU:HA	1:C:22:LEU:HD11	1.86	0.56
1:C:179:GLN:HG3	2:D:157:HIS:O	2.05	0.56
2:D:226:LEU:HB3	2:D:228:VAL:HG22	1.87	0.56
2:F:87:VAL:HG21	2:F:104:LEU:HB3	1.87	0.56
1:H:92:LEU:HB2	1:H:94:LEU:HD12	1.87	0.56
1:H:134:VAL:HG12	1:H:135:PRO:CD	2.35	0.56
2:G:83:ARG:HD3	1:K:84:HIS:HB3	1.87	0.56
1:N:47:SER:OG	1:N:189:LYS:HD2	2.05	0.56
1:O:187:PHE:CD1	1:O:243:VAL:CG1	2.87	0.56
1:Q:240:VAL:O	1:Q:240:VAL:HG23	2.03	0.56
2:G:84:ALA:O	2:G:87:VAL:HG12	2.05	0.56
1:I:117:LEU:HD11	2:L:94:LEU:HD23	1.87	0.56
1:K:66:ALA:HB3	1:K:72:LEU:HD11	1.86	0.56
1:E:17:LEU:HD11	2:F:85:ARG:CZ	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:128:VAL:HG23	2:F:133:VAL:HG23	1.87	0.56
2:J:51:MET:O	2:J:58:ILE:HD11	2.05	0.56
1:B:122:GLY:O	1:B:141:VAL:HG11	2.05	0.56
1:H:73:LEU:HD12	1:H:73:LEU:N	2.19	0.56
2:G:215:SER:HB2	2:G:270:ARG:NE	2.21	0.56
2:G:271:THR:OG1	2:G:273:VAL:HG23	2.05	0.56
1:K:138:LEU:HD23	1:K:140:GLU:OE2	2.05	0.56
1:H:242:GLU:HA	1:H:267:ILE:O	2.05	0.56
2:L:189:VAL:CG1	2:L:250:GLY:HA3	2.36	0.56
1:H:196:THR:H	1:H:205:ALA:HB1	1.71	0.56
1:O:154:LEU:HD23	2:P:177:LEU:HD11	1.87	0.56
2:A:275:PRO:O	2:A:276:ALA:CB	2.54	0.56
2:J:248:VAL:HB	2:J:255:ARG:HG2	1.88	0.56
2:L:77:LEU:HD11	2:L:177:LEU:HD23	1.86	0.56
1:I:168:ARG:HG2	1:I:169:THR:H	1.70	0.56
1:K:154:LEU:O	1:K:154:LEU:HD23	2.06	0.56
1:K:176:LEU:HD13	2:L:158:HIS:CE1	2.41	0.56
2:L:83:ARG:O	2:L:87:VAL:HG23	2.06	0.56
1:O:60:VAL:O	1:O:64:VAL:HG23	2.06	0.56
1:H:138:LEU:HB2	1:H:141:VAL:CG1	2.36	0.55
2:G:235:VAL:O	2:G:238:THR:HG22	2.06	0.55
1:O:67:ARG:NH1	1:O:121:HIS:O	2.38	0.55
1:O:228:PHE:N	1:O:229:PRO:HD2	2.21	0.55
1:I:135:PRO:O	1:I:141:VAL:HG12	2.06	0.55
2:D:124:GLY:O	2:D:144:THR:HG21	2.06	0.55
2:G:68:LEU:HD21	2:G:257:THR:HG23	1.89	0.55
1:C:99:LEU:HD22	1:C:163:VAL:HG12	1.88	0.55
2:J:226:LEU:CD1	2:J:233:LEU:HD11	2.37	0.55
1:N:247:ASN:OD1	1:N:250:VAL:N	2.39	0.55
1:C:246:VAL:CG1	1:C:253:ASN:HB3	2.36	0.55
2:G:96:LEU:HD21	1:K:117:LEU:HD21	1.87	0.55
2:G:199:ASP:HB2	2:G:225:PRO:HG2	1.87	0.55
1:N:31:ASP:OD1	1:N:239:HIS:NE2	2.39	0.55
2:A:191:ASN:OD1	4:A:301:ATP:O3'	2.17	0.55
1:H:95:PRO:O	1:H:98:VAL:HG22	2.06	0.55
1:I:213:VAL:CA	1:I:216:MET:HB2	2.34	0.55
1:B:260:GLY:CA	2:M:205:ARG:NH2	2.69	0.55
2:A:41:LEU:HD12	2:A:73:ARG:O	2.06	0.55
1:H:129:ALA:HB1	2:G:157:HIS:ND1	2.22	0.55
1:I:40:VAL:O	1:I:185:MET:SD	2.65	0.55
1:I:41:ILE:C	1:I:185:MET:HE1	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:50:ASP:OD2	1:K:80:THR:HG23	2.07	0.55
1:N:78:ALA:HB1	1:N:82:ALA:HB2	1.89	0.55
1:O:213:VAL:HG21	1:O:235:GLN:CD	2.27	0.55
2:P:227:PRO:HD3	4:P:301:ATP:C6	2.42	0.55
2:D:193:ASP:HA	2:D:249:ASN:HB2	1.89	0.55
1:H:85:LEU:HD13	1:H:102:LEU:HB3	1.87	0.55
1:I:31:ASP:OD1	1:I:32:PHE:N	2.40	0.55
1:I:168:ARG:HB3	1:I:227:GLU:OE1	2.07	0.55
1:B:223:ASP:HB2	1:B:228:PHE:HB3	1.90	0.55
1:E:252:GLY:O	1:E:256:ARG:HG3	2.07	0.55
1:N:121:HIS:ND1	3:N:302:SO4:O2	2.36	0.55
2:D:264:HIS:NE2	2:D:266:GLY:O	2.40	0.54
1:I:122:GLY:O	1:I:141:VAL:CG2	2.56	0.54
1:N:188:VAL:HG23	1:N:188:VAL:O	2.07	0.54
1:B:101:GLN:HB3	1:B:153:LYS:HB3	1.89	0.54
1:E:11:LEU:O	1:E:15:ARG:HB2	2.08	0.54
1:I:141:VAL:HG12	1:I:142:ASN:N	2.21	0.54
1:K:94:LEU:HB3	1:K:98:VAL:HG21	1.90	0.54
1:N:120:LYS:HG2	1:O:34:ILE:O	2.06	0.54
1:C:50:ASP:OD2	1:C:80:THR:HG23	2.08	0.54
2:R:246:GLN:HG2	2:R:248:VAL:HG13	1.89	0.54
2:P:166:PRO:O	2:P:169:ARG:NH1	2.40	0.54
2:D:273:VAL:HG12	2:D:275:PRO:HD3	1.90	0.54
2:G:248:VAL:HG11	2:G:259:ALA:HB2	1.89	0.54
1:I:116:GLN:O	1:K:34:ILE:HG23	2.07	0.54
1:I:122:GLY:CA	1:K:137:SER:OG	2.55	0.54
2:L:252:VAL:CG2	2:L:255:ARG:HD2	2.30	0.54
1:O:77:GLY:HA2	1:O:169:THR:HG21	1.90	0.54
1:E:194:LEU:HD11	1:E:221:LEU:HD13	1.89	0.54
1:H:30:ALA:O	2:G:95:GLY:HA2	2.08	0.54
1:H:219:LYS:HB3	1:H:221:LEU:CG	2.37	0.54
1:O:190:ASP:CA	1:O:249:LEU:HD23	2.35	0.54
1:B:213:VAL:HG22	1:B:269:ALA:O	2.07	0.54
1:B:225:ILE:HG23	1:B:226:LEU:HG	1.90	0.54
1:E:47:SER:OG	3:E:301:SO4:O2	2.17	0.54
1:H:71:LYS:N	1:H:71:LYS:HD2	2.23	0.54
1:H:196:THR:N	1:H:205:ALA:HB1	2.23	0.54
2:F:83:ARG:NH2	2:F:112:ASN:OD1	2.41	0.54
1:H:241:ARG:HE	1:H:269:ALA:CB	2.21	0.54
1:Q:15:ARG:HD3	1:Q:19:ASP:CG	2.28	0.54
1:B:53:ARG:HG3	1:B:57:TYR:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:81:GLY:O	2:F:85:ARG:NH1	2.41	0.54
1:I:122:GLY:HA2	1:K:137:SER:OG	2.07	0.54
1:B:219:LYS:HB3	1:B:221:LEU:HD23	1.90	0.53
1:K:115:GLY:HA3	1:K:125:VAL:HG13	1.89	0.53
2:L:88:PHE:O	2:L:92:LEU:N	2.30	0.53
1:N:225:ILE:HG23	1:N:226:LEU:HG	1.89	0.53
2:R:198:ALA:H	2:R:208:ALA:HB1	1.72	0.53
1:K:114:LEU:O	1:K:118:LEU:HD13	2.07	0.53
1:C:94:LEU:O	1:C:163:VAL:HG11	2.09	0.53
1:C:148:GLY:O	1:C:172:GLY:HA3	2.09	0.53
1:I:141:VAL:HG12	1:I:142:ASN:H	1.73	0.53
1:O:247:ASN:OD1	1:O:249:LEU:HB2	2.08	0.53
2:P:151:ALA:HB3	2:P:170:ALA:HB1	1.89	0.53
1:Q:217:LYS:HA	1:Q:222:HIS:ND1	2.24	0.53
2:A:191:ASN:HB2	2:A:251:LEU:HD11	1.91	0.53
1:C:5:THR:HG23	1:C:5:THR:O	2.09	0.53
1:I:141:VAL:CG1	1:I:142:ASN:N	2.71	0.53
1:N:50:ASP:OD2	1:N:80:THR:HG23	2.08	0.53
1:N:138:LEU:HD22	1:O:138:LEU:HD21	1.90	0.53
1:N:262:HIS:CD2	1:N:266:ILE:HD12	2.44	0.53
2:P:68:LEU:HD21	2:P:257:THR:HA	1.91	0.53
1:E:17:LEU:HD12	1:E:17:LEU:H	1.73	0.53
2:J:130:HIS:HA	2:J:133:VAL:HG22	1.91	0.53
1:C:140:GLU:OE1	1:E:138:LEU:HD23	2.08	0.53
1:E:76:THR:HG21	1:E:111:ALA:HA	1.90	0.53
1:H:247:ASN:ND2	1:H:248:GLY:O	2.42	0.53
2:J:255:ARG:HG3	2:J:265:VAL:HG21	1.90	0.53
2:L:43:VAL:HG12	2:L:186:LEU:HD13	1.91	0.53
2:L:233:LEU:HA	2:L:236:MET:HE2	1.91	0.53
1:Q:228:PHE:CD1	1:Q:229:PRO:HD3	2.43	0.53
1:H:78:ALA:O	1:H:106:VAL:HG12	2.09	0.53
1:K:67:ARG:O	1:K:142:ASN:HB2	2.09	0.53
1:O:53:ARG:N	2:R:93:ASP:OD2	2.35	0.53
1:O:53:ARG:HB2	2:R:93:ASP:O	2.09	0.53
1:C:8:LEU:O	1:C:12:LEU:N	2.35	0.53
1:C:66:ALA:HB1	1:C:258:LEU:HD13	1.90	0.53
1:K:73:LEU:CD1	1:K:136:LEU:HD21	2.39	0.53
2:L:65:LEU:HD11	2:L:256:LEU:HD23	1.90	0.53
1:B:244:GLN:NE2	1:B:263:VAL:O	2.37	0.53
1:H:17:LEU:HB2	2:G:169:ARG:HH12	1.73	0.53
2:P:37:LEU:N	2:P:181:PHE:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:223:ASP:OD1	1:Q:226:LEU:O	2.26	0.53
2:A:264:HIS:NE2	2:A:266:GLY:O	2.42	0.52
1:K:40:VAL:HG13	1:K:185:MET:SD	2.49	0.52
1:Q:213:VAL:HG21	1:Q:235:GLN:CG	2.39	0.52
2:R:175:PHE:HA	2:R:186:LEU:HD22	1.90	0.52
1:E:52:GLY:O	1:E:56:VAL:HG23	2.09	0.52
1:H:15:ARG:NH1	1:H:21:GLN:HB3	2.25	0.52
1:H:131:LEU:HD22	1:H:131:LEU:O	2.09	0.52
2:G:153:PRO:HD3	2:G:173:GLY:HA3	1.92	0.52
1:K:61:ASP:O	1:K:64:VAL:HG22	2.09	0.52
1:C:17:LEU:HD11	2:D:85:ARG:HD2	1.90	0.52
2:J:144:THR:HG23	2:J:146:ALA:H	1.75	0.52
1:O:17:LEU:HD23	1:O:22:LEU:HD11	1.92	0.52
2:G:45:LYS:HA	2:G:77:LEU:O	2.09	0.52
2:L:45:LYS:HE3	2:L:170:ALA:HB1	1.92	0.52
5:M:302:CL:CL	2:R:140:HIS:NE2	2.68	0.52
1:B:15:ARG:HD2	1:B:19:ASP:OD2	2.10	0.52
1:B:179:GLN:HG3	2:A:157:HIS:O	2.10	0.52
1:B:225:ILE:HG12	1:B:245:VAL:HG11	1.92	0.52
2:A:87:VAL:HG11	2:A:104:LEU:HB3	1.92	0.52
1:E:192:ASP:HA	1:E:247:ASN:HB2	1.92	0.52
1:H:94:LEU:HB3	1:H:98:VAL:CG2	2.38	0.52
1:H:228:PHE:N	1:H:229:PRO:HD2	2.25	0.52
2:G:45:LYS:HG2	2:G:77:LEU:O	2.10	0.52
1:K:98:VAL:HG11	2:L:37:LEU:HD21	1.91	0.52
1:Q:179:GLN:HG3	2:R:157:HIS:O	2.09	0.52
1:B:213:VAL:HG23	1:B:214:ASP:N	2.25	0.52
1:E:12:LEU:HB3	2:F:85:ARG:HB3	1.92	0.52
1:H:118:LEU:HB2	1:H:123:ILE:CG2	2.40	0.52
1:H:179:GLN:HG3	2:G:157:HIS:O	2.09	0.52
2:G:85:ARG:HA	2:G:88:PHE:CD2	2.44	0.52
1:I:155:TRP:NE1	2:J:177:LEU:HD13	2.25	0.52
1:I:208:ILE:HG23	1:I:208:ILE:O	2.10	0.52
1:K:213:VAL:HG23	1:K:214:ASP:N	2.25	0.52
2:L:160:PHE:HB3	2:L:161:PRO:HD2	1.91	0.52
2:L:249:ASN:O	2:L:252:VAL:HG22	2.09	0.52
1:C:30:ALA:O	2:D:95:GLY:HA2	2.09	0.52
1:H:138:LEU:HB2	1:H:141:VAL:HG13	1.92	0.52
1:H:213:VAL:HG23	1:H:214:ASP:N	2.24	0.52
2:G:93:ASP:OD1	1:K:53:ARG:NH2	2.43	0.52
2:R:264:HIS:NE2	2:R:266:GLY:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:214:THR:HG21	2:G:219:LEU:HD11	1.92	0.52
1:I:213:VAL:C	1:I:216:MET:H	2.12	0.52
1:Q:213:VAL:HG21	1:Q:235:GLN:HG2	1.91	0.52
2:A:227:PRO:HD3	4:A:301:ATP:C6	2.45	0.52
1:K:42:LYS:NZ	1:K:170:ASP:OD1	2.40	0.52
1:K:81:ARG:O	1:K:85:LEU:HD12	2.10	0.52
1:K:152:TYR:O	1:K:155:TRP:N	2.42	0.52
1:N:138:LEU:HD11	1:O:134:VAL:HG13	1.92	0.52
1:E:194:LEU:HD11	1:E:221:LEU:CD1	2.41	0.51
1:I:212:SER:N	1:I:215:GLU:OE1	2.42	0.51
1:N:157:ARG:HG2	2:M:176:LEU:HD21	1.93	0.51
2:M:140:HIS:NE2	5:M:302:CL:CL	2.67	0.51
2:R:133:VAL:CG1	2:R:177:LEU:HD21	2.39	0.51
1:B:133:ALA:O	1:B:137:SER:N	2.40	0.51
2:F:86:HIS:O	2:F:90:VAL:HG23	2.09	0.51
1:K:186:ILE:HG22	1:K:187:PHE:H	1.76	0.51
2:L:222:SER:O	2:L:230:ARG:NH2	2.42	0.51
1:N:17:LEU:HA	1:N:22:LEU:HD22	1.92	0.51
2:R:195:ILE:HD12	2:R:267:THR:HG21	1.91	0.51
1:H:77:GLY:O	1:H:110:ASN:ND2	2.43	0.51
1:H:208:ILE:HG23	1:H:208:ILE:O	2.11	0.51
2:G:252:VAL:HG23	2:G:252:VAL:O	2.10	0.51
2:L:45:LYS:CE	2:L:170:ALA:HB1	2.40	0.51
1:N:138:LEU:HD12	1:N:141:VAL:CG2	2.40	0.51
2:R:103:PRO:HB3	2:R:156:HIS:HB3	1.93	0.51
1:H:172:GLY:O	2:G:158:HIS:HE1	1.94	0.51
2:G:143:ALA:HB2	2:J:143:ALA:HB1	1.91	0.51
1:I:48:VAL:O	1:I:56:VAL:HG22	2.09	0.51
1:O:47:SER:OG	1:O:189:LYS:HD2	2.10	0.51
1:E:154:LEU:HD23	2:F:177:LEU:HD11	1.92	0.51
2:J:75:LEU:HG	2:J:77:LEU:HD11	1.93	0.51
1:E:244:GLN:NE2	1:E:263:VAL:O	2.41	0.51
1:I:196:THR:HG22	1:I:196:THR:O	2.10	0.51
1:I:213:VAL:O	1:I:214:ASP:C	2.48	0.51
2:M:80:ALA:HB1	2:M:84:ALA:HB2	1.93	0.51
2:D:196:TYR:HA	2:D:209:ARG:O	2.11	0.51
2:G:46:ILE:HG22	2:G:50:VAL:HG23	1.93	0.51
1:I:123:ILE:HG23	1:I:123:ILE:O	2.11	0.51
1:K:94:LEU:O	1:K:163:VAL:HG11	2.10	0.51
2:R:37:LEU:N	2:R:181:PHE:O	2.43	0.51
2:G:84:ALA:O	2:G:88:PHE:CD1	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:271:THR:OG1	2:J:273:VAL:HG23	2.10	0.51
2:P:88:PHE:CE1	2:P:105:ALA:HB2	2.46	0.51
1:C:66:ALA:CB	1:C:258:LEU:HD13	2.40	0.51
1:C:138:LEU:CD1	1:C:138:LEU:N	2.73	0.51
1:C:152:TYR:O	1:C:155:TRP:N	2.44	0.51
1:H:252:GLY:O	1:H:256:ARG:HG2	2.11	0.51
2:G:88:PHE:CD2	2:G:165:ILE:HD11	2.46	0.51
1:B:62:GLU:OE1	1:B:255:THR:OG1	2.29	0.50
2:D:144:THR:HG22	2:D:145:ARG:N	2.25	0.50
1:K:67:ARG:HG3	1:K:141:VAL:O	2.11	0.50
1:K:76:THR:HG21	1:K:111:ALA:CA	2.41	0.50
1:Q:22:LEU:HD23	1:Q:22:LEU:O	2.11	0.50
1:Q:154:LEU:HD23	2:R:177:LEU:HD11	1.93	0.50
1:Q:200:LYS:HG3	1:Q:201:THR:HG23	1.93	0.50
1:B:68:LYS:HD3	1:I:256:ARG:NH1	2.26	0.50
1:B:252:GLY:O	1:B:256:ARG:HG2	2.11	0.50
1:C:192:ASP:HB3	1:C:207:PHE:HE2	1.76	0.50
1:H:195:TYR:HB3	1:H:205:ALA:CB	2.41	0.50
2:L:55:ALA:O	2:L:59:LEU:HD12	2.11	0.50
2:L:65:LEU:HD23	2:L:76:ILE:HD13	1.93	0.50
1:N:183:LYS:HG3	1:N:184:GLN:HG3	1.93	0.50
1:Q:247:ASN:OD1	1:Q:250:VAL:HG23	2.12	0.50
1:C:213:VAL:HG21	1:C:235:GLN:HG2	1.93	0.50
1:C:265:THR:HG22	1:C:266:ILE:N	2.27	0.50
1:I:108:ASP:OD1	1:I:147:SER:OG	2.11	0.50
1:I:222:HIS:O	1:I:223:ASP:C	2.48	0.50
1:I:216:MET:O	1:I:221:LEU:HB2	2.11	0.50
1:K:13:MET:O	2:L:49:ARG:NH1	2.44	0.50
1:K:18:THR:HG22	2:L:230:ARG:HG3	1.94	0.50
1:O:50:ASP:OD2	1:O:80:THR:HG23	2.11	0.50
1:H:80:THR:HG23	1:H:81:ARG:N	2.27	0.50
2:G:197:THR:CG2	2:G:211:LEU:HD11	2.41	0.50
1:K:93:GLY:O	2:L:35:ILE:N	2.42	0.50
1:Q:50:ASP:OD2	1:Q:80:THR:HG23	2.11	0.50
1:I:40:VAL:HA	1:I:73:LEU:O	2.12	0.50
1:N:170:ASP:HB2	1:N:227:GLU:OE1	2.12	0.50
2:R:63:GLU:O	2:R:67:LYS:HG2	2.12	0.50
1:B:138:LEU:HD23	1:E:140:GLU:OE2	2.12	0.50
1:E:60:VAL:O	1:E:64:VAL:HG23	2.12	0.50
1:E:78:ALA:HB1	1:E:82:ALA:HB2	1.93	0.50
1:H:101:GLN:HG2	1:H:153:LYS:HB3	1.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:221:LEU:CD1	1:H:221:LEU:N	2.74	0.50
1:I:247:ASN:HD21	1:I:249:LEU:HD23	1.77	0.50
2:M:136:GLN:OE1	2:P:128:VAL:HG12	2.12	0.50
1:Q:228:PHE:CG	1:Q:229:PRO:HD3	2.46	0.50
1:K:208:ILE:HD13	1:K:211:ILE:HD12	1.94	0.50
1:O:217:LYS:HG2	1:O:222:HIS:ND1	2.27	0.50
2:P:80:ALA:HB1	2:P:84:ALA:HB2	1.93	0.50
2:G:103:PRO:HB3	2:G:156:HIS:CG	2.47	0.49
2:J:77:LEU:HD23	2:J:151:ALA:HA	1.93	0.49
1:K:228:PHE:N	1:K:229:PRO:HD2	2.27	0.49
1:C:196:THR:HG22	1:C:221:LEU:HD11	1.93	0.49
1:H:80:THR:HG21	2:J:86:HIS:CE1	2.47	0.49
1:H:172:GLY:O	2:G:158:HIS:CE1	2.66	0.49
2:G:175:PHE:CE2	2:G:236:MET:HG2	2.47	0.49
1:K:81:ARG:NE	1:K:109:GLN:OE1	2.44	0.49
1:C:78:ALA:HB1	1:C:82:ALA:CB	2.43	0.49
1:C:175:LEU:HD13	2:D:158:HIS:O	2.12	0.49
1:H:48:VAL:HG11	1:H:59:LEU:HD11	1.93	0.49
1:H:226:LEU:HD12	1:H:231:LEU:CD2	2.35	0.49
2:G:232:LEU:HD11	2:G:236:MET:HE3	1.94	0.49
1:I:157:ARG:HG2	2:J:176:LEU:HD21	1.94	0.49
2:J:77:LEU:N	2:J:77:LEU:HD12	2.27	0.49
1:O:234:LEU:HG	1:O:269:ALA:HB2	1.94	0.49
1:Q:225:ILE:HG23	1:Q:226:LEU:HD13	1.93	0.49
1:E:33:ARG:NH2	1:E:239:HIS:O	2.45	0.49
2:G:103:PRO:HD3	2:G:156:HIS:O	2.12	0.49
2:G:120:LEU:HD22	2:G:125:VAL:HG21	1.93	0.49
1:C:135:PRO:HB2	1:C:144:VAL:HG12	1.95	0.49
1:C:213:VAL:HG23	1:C:214:ASP:N	2.28	0.49
1:I:105:SER:O	1:I:109:GLN:N	2.39	0.49
1:K:195:TYR:HB3	1:K:205:ALA:HB1	1.94	0.49
2:D:239:ALA:O	2:D:273:VAL:CG2	2.58	0.49
1:E:220:GLY:HA2	1:E:222:HIS:CE1	2.47	0.49
2:G:52:ASP:OD2	2:G:82:VAL:HG12	2.12	0.49
2:G:77:LEU:HB3	2:G:151:ALA:HB2	1.95	0.49
1:I:151:PRO:HB2	2:J:154:PRO:O	2.11	0.49
1:K:186:ILE:HG22	1:K:187:PHE:N	2.27	0.49
2:D:37:LEU:N	2:D:181:PHE:O	2.45	0.49
1:E:211:ILE:CD1	1:E:216:MET:HG2	2.42	0.49
2:F:43:VAL:HG12	2:F:186:LEU:HD13	1.94	0.49
1:H:175:LEU:HD13	2:G:158:HIS:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:VAL:HG23	1:B:214:ASP:H	1.78	0.49
2:F:33:ARG:N	2:F:240:ARG:NH2	2.60	0.49
2:G:43:VAL:HG11	2:G:178:ALA:CB	2.42	0.49
1:K:13:MET:H	1:K:13:MET:CE	2.26	0.49
1:K:101:GLN:HB3	1:K:153:LYS:HB3	1.95	0.49
1:H:61:ASP:O	1:H:64:VAL:HG22	2.13	0.49
2:G:88:PHE:O	2:G:92:LEU:N	2.37	0.49
1:I:78:ALA:H	1:I:168:ARG:NH2	2.11	0.49
2:L:82:VAL:HG13	2:L:83:ARG:N	2.26	0.49
1:N:152:TYR:O	1:N:155:TRP:N	2.46	0.49
1:Q:5:THR:O	1:Q:5:THR:HG23	2.13	0.49
1:Q:10:GLU:OE1	1:Q:13:MET:HE3	2.13	0.49
1:H:192:ASP:O	1:H:264:GLY:HA2	2.12	0.49
1:I:85:LEU:HD21	2:L:83:ARG:CZ	2.43	0.49
1:I:222:HIS:O	1:I:224:SER:OG	2.24	0.49
2:M:103:PRO:HB3	2:M:156:HIS:HB3	1.94	0.49
1:H:226:LEU:CD1	1:H:267:ILE:HD13	2.31	0.48
2:G:88:PHE:HE1	2:G:105:ALA:HB2	1.78	0.48
1:K:17:LEU:N	1:K:17:LEU:HD12	2.28	0.48
1:K:193:GLY:HA2	1:K:245:VAL:HG12	1.94	0.48
2:D:80:ALA:HB1	2:D:84:ALA:HB2	1.94	0.48
1:I:237:ALA:HA	2:J:161:PRO:HB2	1.93	0.48
2:J:88:PHE:CE1	2:J:101:LEU:HB3	2.48	0.48
1:K:111:ALA:O	1:K:125:VAL:HG11	2.12	0.48
2:P:199:ASP:OD2	2:P:202:GLY:N	2.46	0.48
1:B:228:PHE:N	1:B:229:PRO:HD2	2.29	0.48
1:C:219:LYS:O	1:C:219:LYS:HG3	2.13	0.48
1:N:42:LYS:O	1:N:188:VAL:HG22	2.12	0.48
1:N:172:GLY:HA2	2:M:158:HIS:CD2	2.48	0.48
2:M:62:VAL:HG13	2:M:120:LEU:HG	1.95	0.48
1:O:217:LYS:NZ	1:O:222:HIS:CE1	2.81	0.48
1:Q:138:LEU:N	1:Q:138:LEU:HD12	2.28	0.48
1:B:106:VAL:HA	1:B:109:GLN:HE21	1.78	0.48
1:E:123:ILE:HG12	1:E:143:ALA:HB3	1.96	0.48
1:E:220:GLY:HA2	1:E:222:HIS:HE1	1.78	0.48
1:H:17:LEU:CB	2:G:169:ARG:HH12	2.25	0.48
2:G:133:VAL:HA	2:G:137:LEU:CD1	2.43	0.48
1:Q:219:LYS:O	1:Q:219:LYS:HG3	2.13	0.48
1:H:5:THR:HG23	1:H:6:ALA:N	2.29	0.48
1:O:250:VAL:HB	1:O:253:ASN:ND2	2.27	0.48
2:R:196:TYR:HD2	2:R:208:ALA:O	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:GLU:O	1:B:218:ALA:HB3	2.14	0.48
1:C:190:ASP:CA	1:C:249:LEU:HD23	2.44	0.48
2:D:214:THR:O	2:D:269:ILE:HA	2.13	0.48
2:G:88:PHE:CE2	2:G:165:ILE:HD11	2.48	0.48
2:J:88:PHE:HB3	2:J:92:LEU:HD12	1.94	0.48
1:K:254:LEU:C	1:K:254:LEU:HD23	2.33	0.48
1:O:52:GLY:O	1:O:56:VAL:HG23	2.14	0.48
1:O:85:LEU:HD21	2:R:83:ARG:CZ	2.44	0.48
1:O:230:VAL:O	1:O:234:LEU:N	2.46	0.48
2:D:75:LEU:CD1	2:D:147:VAL:HG23	2.44	0.48
1:H:223:ASP:CG	1:H:228:PHE:HB3	2.32	0.48
2:G:220:ALA:HA	2:G:233:LEU:HD23	1.96	0.48
1:I:85:LEU:HD21	2:L:83:ARG:NE	2.29	0.48
1:K:149:MET:SD	1:K:150:PRO:HD2	2.54	0.48
1:K:163:VAL:CG1	1:K:163:VAL:O	2.61	0.48
1:C:237:ALA:O	1:C:241:ARG:CD	2.62	0.48
2:D:226:LEU:CB	2:D:228:VAL:HG22	2.44	0.48
2:F:52:ASP:OD2	2:F:82:VAL:HG12	2.14	0.48
2:G:83:ARG:NH1	1:K:85:LEU:HG	2.28	0.48
2:L:243:GLU:HA	2:L:271:THR:OG1	2.13	0.48
1:C:60:VAL:O	1:C:64:VAL:HG23	2.14	0.48
1:I:48:VAL:O	1:I:48:VAL:HG12	2.13	0.48
1:B:202:SER:HB2	1:B:205:ALA:HB2	1.95	0.48
1:C:100:ALA:HB3	1:C:153:LYS:O	2.14	0.48
2:D:78:THR:HG21	2:D:113:GLY:HA2	1.96	0.48
1:H:8:LEU:HD11	1:H:26:ALA:HA	1.95	0.48
1:H:95:PRO:O	1:H:99:LEU:HD13	2.14	0.48
1:H:125:VAL:HG21	1:I:131:LEU:HB3	1.96	0.48
1:H:195:TYR:HB3	1:H:205:ALA:HB1	1.96	0.48
2:J:128:VAL:CG2	2:J:133:VAL:HG12	2.42	0.48
1:Q:8:LEU:HA	1:Q:11:LEU:HB2	1.96	0.48
1:Q:257:ALA:HB2	1:Q:263:VAL:HG22	1.95	0.48
1:B:78:ALA:HB1	1:B:82:ALA:CB	2.44	0.47
1:C:34:ILE:O	1:C:35:LEU:HD23	2.14	0.47
2:D:264:HIS:CD2	2:D:266:GLY:O	2.67	0.47
1:E:20:PRO:HA	1:E:23:GLN:HB2	1.96	0.47
1:H:194:LEU:HD21	1:H:224:SER:HB3	1.95	0.47
1:I:40:VAL:HG11	1:I:177:ALA:HB2	1.95	0.47
1:I:100:ALA:HB3	1:I:153:LYS:HA	1.95	0.47
2:J:63:GLU:OE2	2:J:66:ARG:NH2	2.47	0.47
2:L:214:THR:HG21	2:L:219:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:195:TYR:CD1	1:N:207:PHE:HA	2.48	0.47
2:M:139:ILE:O	2:M:143:ALA:N	2.47	0.47
1:O:262:HIS:O	1:O:262:HIS:CG	2.67	0.47
1:B:78:ALA:HB1	1:B:82:ALA:HB2	1.96	0.47
2:A:110:GLY:O	2:A:114:HIS:ND1	2.39	0.47
2:A:143:ALA:HB2	2:D:143:ALA:HB1	1.96	0.47
1:N:89:ALA:HB1	1:N:94:LEU:HD12	1.96	0.47
1:N:138:LEU:HD12	1:N:141:VAL:HG21	1.97	0.47
1:Q:192:ASP:O	1:Q:264:GLY:HA2	2.14	0.47
1:Q:197:ALA:HB3	1:Q:205:ALA:HB2	1.96	0.47
1:H:8:LEU:HA	1:H:11:LEU:HB2	1.95	0.47
1:H:208:ILE:O	1:H:208:ILE:CG2	2.61	0.47
1:H:223:ASP:OD1	1:H:228:PHE:CB	2.63	0.47
1:I:124:PRO:HG3	1:K:134:VAL:HG23	1.96	0.47
1:N:67:ARG:HE	1:N:68:LYS:NZ	2.12	0.47
2:M:63:GLU:O	2:M:67:LYS:HG2	2.14	0.47
2:G:44:VAL:HG11	2:G:256:LEU:HD21	1.96	0.47
2:G:93:ASP:O	1:K:53:ARG:NH2	2.47	0.47
2:G:228:VAL:HB	2:G:232:LEU:HD23	1.97	0.47
2:G:235:VAL:O	2:G:238:THR:N	2.45	0.47
1:I:17:LEU:HD11	2:J:85:ARG:NE	2.29	0.47
2:J:129:GLU:O	2:J:133:VAL:HG13	2.14	0.47
1:N:104:SER:HA	1:N:149:MET:HG3	1.97	0.47
2:P:144:THR:HG23	2:P:146:ALA:H	1.79	0.47
2:P:273:VAL:HG12	2:P:274:ARG:N	2.29	0.47
1:E:9:GLU:O	1:E:13:MET:HG2	2.14	0.47
1:E:223:ASP:OD1	1:E:226:LEU:O	2.32	0.47
2:F:144:THR:HG23	2:F:146:ALA:H	1.79	0.47
1:H:114:LEU:O	1:H:118:LEU:HG	2.15	0.47
1:I:6:ALA:O	1:I:10:GLU:CD	2.53	0.47
2:J:88:PHE:O	2:J:92:LEU:HB2	2.14	0.47
1:K:39:THR:HG21	1:K:258:LEU:CD2	2.44	0.47
1:K:66:ALA:HB1	1:K:72:LEU:HD21	1.97	0.47
1:E:17:LEU:O	1:E:23:GLN:NE2	2.32	0.47
1:E:99:LEU:HD22	1:E:163:VAL:HG12	1.97	0.47
1:K:236:SER:HB2	2:L:161:PRO:HG2	1.97	0.47
1:N:247:ASN:OD1	1:N:250:VAL:HG23	2.15	0.47
1:O:134:VAL:HB	1:O:135:PRO:HD3	1.96	0.47
1:O:221:LEU:HD23	1:O:224:SER:OG	2.14	0.47
1:C:89:ALA:HB1	1:C:94:LEU:HD12	1.97	0.47
1:C:171:ALA:HB2	1:C:230:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:248:VAL:HG11	2:D:259:ALA:HB2	1.97	0.47
1:E:17:LEU:HD12	1:E:17:LEU:N	2.29	0.47
1:E:170:ASP:HB2	1:E:227:GLU:OE1	2.15	0.47
2:G:47:GLY:O	2:G:50:VAL:HG22	2.14	0.47
2:G:169:ARG:HB2	2:G:229:ASP:OD2	2.15	0.47
1:I:63:ILE:HD13	1:I:254:LEU:HD21	1.96	0.47
1:K:101:GLN:HB3	1:K:153:LYS:CB	2.45	0.47
2:L:246:GLN:HG2	2:L:248:VAL:HG13	1.96	0.47
1:O:10:GLU:O	1:O:14:GLN:HB2	2.14	0.47
1:Q:246:VAL:CG1	1:Q:247:ASN:N	2.78	0.47
1:I:185:MET:HE3	1:I:187:PHE:CD1	2.50	0.47
1:I:188:VAL:HG23	1:I:188:VAL:O	2.15	0.47
2:L:273:VAL:HG12	2:L:274:ARG:N	2.30	0.47
1:N:30:ALA:O	2:M:95:GLY:HA2	2.15	0.47
1:O:227:GLU:C	1:O:229:PRO:HD2	2.35	0.47
1:H:34:ILE:HD12	1:K:116:GLN:O	2.14	0.47
1:H:252:GLY:O	1:H:256:ARG:CG	2.62	0.47
2:G:197:THR:N	2:G:209:ARG:O	2.45	0.47
1:N:195:TYR:CD1	1:N:205:ALA:O	2.68	0.47
1:B:152:TYR:HB3	1:B:156:MET:HA	1.97	0.47
2:L:252:VAL:O	2:L:252:VAL:CG2	2.62	0.47
1:N:228:PHE:CG	1:N:229:PRO:HD3	2.50	0.47
1:B:135:PRO:HB2	1:B:144:VAL:CG1	2.46	0.46
1:B:227:GLU:HB2	1:B:230:VAL:HG23	1.98	0.46
2:G:88:PHE:CG	2:G:165:ILE:HD11	2.50	0.46
2:G:120:LEU:HD23	2:G:120:LEU:O	2.15	0.46
1:I:50:ASP:OD2	1:I:80:THR:HG23	2.15	0.46
1:I:117:LEU:HA	1:K:32:PHE:CE2	2.51	0.46
1:I:213:VAL:O	1:I:217:LYS:N	2.47	0.46
1:N:78:ALA:HB1	1:N:82:ALA:CB	2.45	0.46
1:Q:203:LYS:CG	1:Q:204:ASP:N	2.77	0.46
2:A:41:LEU:HD12	2:A:42:GLN:N	2.30	0.46
1:C:194:LEU:O	1:C:195:TYR:HD1	1.98	0.46
1:E:228:PHE:CD1	1:E:229:PRO:HD3	2.50	0.46
1:H:158:PRO:HD2	2:G:238:THR:HG21	1.98	0.46
1:H:221:LEU:C	1:H:223:ASP:N	2.55	0.46
2:J:272:GLY:HA2	2:J:274:ARG:NH2	2.31	0.46
1:K:30:ALA:O	2:L:95:GLY:HA2	2.15	0.46
1:K:81:ARG:HB2	1:K:106:VAL:CG1	2.46	0.46
1:K:140:GLU:HG2	1:K:141:VAL:HG12	1.97	0.46
1:K:188:VAL:CG2	1:K:188:VAL:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:VAL:O	1:K:188:VAL:HG23	2.15	0.46
1:K:223:ASP:OD1	1:K:226:LEU:O	2.33	0.46
1:N:188:VAL:HG12	1:N:246:VAL:HG23	1.96	0.46
1:N:228:PHE:CD1	1:N:229:PRO:HD3	2.50	0.46
1:Q:226:LEU:HD11	1:Q:245:VAL:CG2	2.46	0.46
2:A:87:VAL:HG22	1:E:81:ARG:CD	2.44	0.46
2:D:151:ALA:HB3	2:D:170:ALA:HB1	1.96	0.46
1:E:72:LEU:O	1:E:143:ALA:HA	2.15	0.46
1:H:46:GLN:HG3	1:H:79:GLY:HA2	1.98	0.46
1:K:42:LYS:HE3	1:K:169:THR:HB	1.96	0.46
2:L:214:THR:O	2:L:269:ILE:HA	2.15	0.46
2:F:248:VAL:HG12	2:F:265:VAL:HG23	1.97	0.46
2:J:117:ALA:HB1	2:J:126:SER:HA	1.97	0.46
2:J:264:HIS:CD2	2:J:266:GLY:O	2.68	0.46
2:L:214:THR:CG2	2:L:219:LEU:HG	2.46	0.46
2:R:198:ALA:H	2:R:208:ALA:CB	2.29	0.46
1:C:39:THR:OG1	1:C:184:GLN:OE1	2.34	0.46
1:C:150:PRO:HD3	1:C:172:GLY:HA3	1.98	0.46
2:G:88:PHE:O	2:G:92:LEU:HB2	2.16	0.46
1:O:243:VAL:CG1	1:O:244:GLN:H	2.28	0.46
2:P:43:VAL:HG12	2:P:186:LEU:HD13	1.98	0.46
1:B:81:ARG:CD	2:D:87:VAL:HG22	2.46	0.46
1:B:138:LEU:HD21	1:E:138:LEU:CD1	2.45	0.46
2:D:172:THR:OG1	2:D:232:LEU:N	2.48	0.46
2:G:111:GLN:HG3	1:K:105:SER:HB3	1.97	0.46
2:G:215:SER:HB2	2:G:270:ARG:HE	1.80	0.46
1:N:228:PHE:N	1:N:229:PRO:HD2	2.30	0.46
2:A:93:ASP:O	1:E:53:ARG:NH1	2.48	0.46
1:H:41:ILE:HD11	1:H:74:ILE:HG12	1.98	0.46
2:G:111:GLN:CG	1:K:105:SER:HB3	2.45	0.46
1:I:47:SER:HB2	1:I:190:ASP:N	2.30	0.46
1:I:214:ASP:OD1	1:I:214:ASP:N	2.48	0.46
1:K:123:ILE:HG12	1:K:141:VAL:HG23	1.97	0.46
1:O:174:PHE:HE2	1:O:233:LEU:HB3	1.81	0.46
1:Q:247:ASN:OD1	1:Q:250:VAL:N	2.49	0.46
2:A:139:ILE:HG22	2:A:140:HIS:N	2.30	0.46
1:H:196:THR:OG1	1:H:205:ALA:HA	2.16	0.46
2:L:233:LEU:HA	2:L:236:MET:CE	2.46	0.46
2:M:166:PRO:O	2:M:169:ARG:NH1	2.48	0.46
1:Q:195:TYR:HB3	1:Q:205:ALA:HB1	1.97	0.46
1:H:216:MET:CE	1:H:224:SER:N	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:PRO:HD3	1:I:172:GLY:HA3	1.98	0.46
2:J:96:LEU:O	2:J:164:ARG:NH2	2.49	0.46
1:K:39:THR:HG21	1:K:258:LEU:HD21	1.97	0.46
1:K:73:LEU:HD12	1:K:136:LEU:HD21	1.98	0.46
1:K:185:MET:HG3	1:K:243:VAL:HG12	1.98	0.46
1:O:213:VAL:HG23	1:O:214:ASP:H	1.80	0.46
1:B:124:PRO:HG3	1:C:134:VAL:CG2	2.46	0.46
2:A:88:PHE:O	2:A:92:LEU:N	2.39	0.46
1:C:126:VAL:HG23	1:C:126:VAL:O	2.14	0.46
1:H:163:VAL:O	1:H:163:VAL:CG1	2.64	0.46
2:G:193:ASP:HA	2:G:249:ASN:HB2	1.98	0.46
1:I:55:ALA:O	1:I:59:LEU:CD1	2.64	0.46
1:I:101:GLN:OE1	1:I:153:LYS:HD3	2.16	0.46
1:I:122:GLY:HA3	1:K:137:SER:CB	2.45	0.46
1:I:163:VAL:HG12	1:I:163:VAL:O	2.16	0.46
2:M:193:ASP:HA	2:M:249:ASN:HB2	1.98	0.46
2:P:257:THR:O	2:P:261:ARG:HG3	2.16	0.46
2:A:129:GLU:O	2:A:133:VAL:HG23	2.17	0.45
2:D:176:LEU:HG	2:D:235:VAL:HG11	1.99	0.45
1:E:41:ILE:HA	1:E:186:ILE:O	2.16	0.45
1:H:40:VAL:HB	1:H:177:ALA:HB2	1.97	0.45
1:H:254:LEU:C	1:H:254:LEU:HD23	2.36	0.45
2:J:257:THR:O	2:J:261:ARG:HG3	2.16	0.45
2:J:275:PRO:O	2:J:276:ALA:CB	2.64	0.45
1:Q:104:SER:HA	1:Q:149:MET:HG3	1.98	0.45
1:Q:228:PHE:N	1:Q:229:PRO:HD2	2.31	0.45
1:C:139:ALA:HA	1:C:142:ASN:OD1	2.16	0.45
2:D:130:HIS:NE2	2:D:152:PHE:O	2.49	0.45
1:H:70:HIS:CD2	1:H:258:LEU:HB3	2.52	0.45
2:G:215:SER:HB2	2:G:270:ARG:CZ	2.46	0.45
1:I:45:GLY:O	1:I:49:ILE:HB	2.15	0.45
2:J:248:VAL:HG12	2:J:265:VAL:HG23	1.97	0.45
1:O:47:SER:O	1:O:51:ARG:NE	2.49	0.45
1:O:213:VAL:HG21	1:O:235:GLN:CG	2.46	0.45
1:Q:138:LEU:HD12	1:Q:138:LEU:H	1.80	0.45
2:R:45:LYS:HA	2:R:77:LEU:O	2.16	0.45
1:B:138:LEU:HB2	1:B:141:VAL:HG23	1.97	0.45
2:A:264:HIS:CD2	2:A:266:GLY:O	2.69	0.45
1:C:77:GLY:HA2	1:C:169:THR:HG21	1.97	0.45
1:H:16:SER:CB	2:G:225:PRO:HB3	2.47	0.45
2:L:68:LEU:HD21	2:L:257:THR:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:219:LYS:HB3	1:O:219:LYS:HE3	1.74	0.45
1:H:78:ALA:HB1	1:H:82:ALA:HB2	1.97	0.45
1:H:221:LEU:HB3	1:H:224:SER:HB2	1.99	0.45
1:I:43:ILE:HD13	1:I:188:VAL:HG22	1.98	0.45
1:I:254:LEU:O	1:I:258:LEU:HG	2.17	0.45
1:K:40:VAL:HA	1:K:73:LEU:O	2.17	0.45
1:K:66:ALA:O	1:K:70:HIS:N	2.49	0.45
1:K:97:GLY:O	1:K:153:LYS:O	2.34	0.45
1:K:240:VAL:O	1:K:240:VAL:HG13	2.17	0.45
2:L:65:LEU:HD23	2:L:76:ILE:CD1	2.46	0.45
1:N:175:LEU:HD13	2:M:158:HIS:O	2.16	0.45
1:B:131:LEU:CD2	1:E:116:GLN:HG2	2.47	0.45
2:D:198:ALA:HB3	2:D:208:ALA:HA	1.97	0.45
1:E:171:ALA:HB2	1:E:230:VAL:HG22	1.99	0.45
1:K:66:ALA:CB	1:K:72:LEU:HD11	2.47	0.45
1:K:123:ILE:HD13	1:K:143:ALA:HB3	1.98	0.45
1:Q:243:VAL:HG23	1:Q:267:ILE:HB	1.98	0.45
2:R:196:TYR:CD1	2:R:200:PRO:HG3	2.51	0.45
2:F:45:LYS:HA	2:F:77:LEU:O	2.17	0.45
1:H:213:VAL:HG23	1:H:214:ASP:H	1.81	0.45
1:H:243:VAL:HG12	1:H:244:GLN:H	1.81	0.45
1:I:123:ILE:CD1	1:I:143:ALA:HB1	2.47	0.45
1:I:262:HIS:CG	1:I:262:HIS:O	2.70	0.45
1:O:11:LEU:HD23	1:O:11:LEU:O	2.16	0.45
2:P:264:HIS:CD2	2:P:266:GLY:O	2.70	0.45
1:C:18:THR:CG2	2:D:230:ARG:HG3	2.46	0.45
1:C:246:VAL:HG12	1:C:247:ASN:N	2.31	0.45
2:F:264:HIS:CD2	2:F:266:GLY:O	2.70	0.45
1:H:92:LEU:HD21	2:J:58:ILE:CD1	2.47	0.45
1:H:179:GLN:O	2:G:97:PRO:HG3	2.16	0.45
1:I:139:ALA:HA	1:I:142:ASN:ND2	2.31	0.45
1:I:148:GLY:O	1:I:172:GLY:HA3	2.17	0.45
1:I:213:VAL:O	1:I:216:MET:CA	2.62	0.45
1:K:154:LEU:CD2	2:L:177:LEU:HD12	2.42	0.45
2:G:217:THR:HG23	2:G:218:ASP:N	2.32	0.45
1:I:118:LEU:HB3	1:I:123:ILE:HG21	1.99	0.45
1:K:8:LEU:HA	1:K:11:LEU:HB2	1.99	0.45
1:K:77:GLY:HA2	1:K:169:THR:HG21	1.97	0.45
1:O:213:VAL:HG23	1:O:214:ASP:N	2.31	0.45
2:P:195:ILE:HG12	2:P:227:PRO:CG	2.47	0.45
1:B:213:VAL:HG21	1:B:235:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:185:MET:CB	1:H:243:VAL:HG13	2.46	0.45
2:G:215:SER:OG	2:G:217:THR:HG22	2.17	0.45
1:K:34:ILE:HD12	1:K:180:PHE:HD1	1.82	0.45
1:N:195:TYR:HB3	1:N:205:ALA:O	2.17	0.45
2:M:88:PHE:CE1	2:M:105:ALA:HB2	2.52	0.45
1:Q:22:LEU:HD22	2:R:165:ILE:HD11	1.99	0.45
1:B:198:ASN:O	1:B:202:SER:HB3	2.17	0.45
1:C:210:ARG:HH11	1:C:266:ILE:HD12	1.82	0.45
2:G:143:ALA:HB2	2:J:143:ALA:CB	2.47	0.45
1:K:8:LEU:C	1:K:10:GLU:N	2.69	0.45
1:K:47:SER:CB	1:K:189:LYS:HG2	2.47	0.45
1:O:97:GLY:O	1:O:153:LYS:O	2.35	0.45
2:A:82:VAL:HA	2:A:85:ARG:HG2	1.99	0.44
2:D:75:LEU:HD13	2:D:147:VAL:HG23	1.99	0.44
1:H:41:ILE:HA	1:H:186:ILE:O	2.16	0.44
2:G:273:VAL:HG12	2:G:274:ARG:N	2.33	0.44
2:J:159:GLU:OE2	2:J:159:GLU:HA	2.17	0.44
2:A:274:ARG:HE	2:A:274:ARG:N	2.14	0.44
1:H:113:MET:HG3	2:J:104:LEU:CD1	2.45	0.44
1:H:248:GLY:C	1:H:249:LEU:HD22	2.37	0.44
2:G:139:ILE:CD1	2:J:147:VAL:HG12	2.47	0.44
1:I:8:LEU:O	1:I:12:LEU:N	2.46	0.44
1:I:42:LYS:HZ3	1:I:189:LYS:HD2	1.83	0.44
2:J:81:GLY:O	2:J:85:ARG:HD2	2.18	0.44
1:N:8:LEU:HD22	1:N:12:LEU:HG	1.99	0.44
1:B:138:LEU:HD21	1:E:138:LEU:HD13	2.00	0.44
2:A:179:ASP:OD2	2:A:239:ALA:HA	2.16	0.44
1:C:11:LEU:HG	1:C:15:ARG:HD2	1.98	0.44
1:C:122:GLY:HA3	1:E:137:SER:HB2	1.99	0.44
1:K:9:GLU:HA	1:K:13:MET:CE	2.47	0.44
1:K:217:LYS:HG2	1:K:228:PHE:CE1	2.52	0.44
1:N:154:LEU:HD23	2:M:177:LEU:HD11	1.99	0.44
2:M:159:GLU:OE2	2:M:168:HIS:ND1	2.43	0.44
1:Q:8:LEU:O	1:Q:12:LEU:N	2.41	0.44
2:R:130:HIS:NE2	2:R:152:PHE:O	2.48	0.44
2:A:83:ARG:O	2:A:87:VAL:HG23	2.17	0.44
1:H:55:ALA:CB	1:H:249:LEU:HD11	2.47	0.44
1:I:105:SER:O	1:I:109:GLN:HG3	2.17	0.44
1:I:242:GLU:HG3	1:I:268:THR:HA	2.00	0.44
2:J:213:GLU:HG2	2:J:268:LEU:HB2	2.00	0.44
2:L:65:LEU:HD11	2:L:256:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:245:VAL:O	2:L:269:ILE:N	2.47	0.44
1:N:134:VAL:N	1:N:135:PRO:CD	2.79	0.44
2:R:86:HIS:O	2:R:90:VAL:HG23	2.17	0.44
1:C:170:ASP:HB2	1:C:227:GLU:OE1	2.17	0.44
1:C:192:ASP:O	1:C:264:GLY:HA2	2.17	0.44
1:C:247:ASN:O	1:C:253:ASN:HB2	2.18	0.44
1:E:163:VAL:O	1:E:163:VAL:CG1	2.65	0.44
1:E:228:PHE:CG	1:E:229:PRO:HD3	2.52	0.44
1:H:56:VAL:CG1	1:H:57:TYR:N	2.80	0.44
2:J:128:VAL:HG22	2:J:148:VAL:O	2.17	0.44
1:K:81:ARG:HB2	1:K:106:VAL:HG13	2.00	0.44
1:K:176:LEU:HD12	1:K:176:LEU:HA	1.92	0.44
2:L:41:LEU:HD12	2:L:183:ALA:HA	1.99	0.44
1:N:46:GLN:OE1	1:N:83:ARG:NE	2.41	0.44
2:D:151:ALA:O	2:D:173:GLY:HA3	2.17	0.44
2:F:84:ALA:O	2:F:87:VAL:HG12	2.17	0.44
2:F:128:VAL:HG23	2:F:133:VAL:CG2	2.48	0.44
1:H:38:ALA:HA	1:H:71:LYS:HB2	1.99	0.44
1:H:219:LYS:CB	1:H:221:LEU:HD13	2.47	0.44
1:I:17:LEU:HA	1:I:22:LEU:HD22	2.00	0.44
2:J:159:GLU:HG3	2:J:167:PRO:HD2	1.99	0.44
2:J:245:VAL:O	2:J:269:ILE:N	2.41	0.44
2:P:241:HIS:O	2:P:275:PRO:HB3	2.18	0.44
1:Q:152:TYR:O	1:Q:155:TRP:N	2.51	0.44
1:Q:225:ILE:HG12	1:Q:245:VAL:HG11	2.00	0.44
1:C:116:GLN:O	1:E:34:ILE:HG23	2.18	0.44
1:E:73[A]:LEU:HD11	1:E:136:LEU:HD11	2.00	0.44
1:H:77:GLY:HA2	1:H:169:THR:HG21	1.99	0.44
1:H:85:LEU:HD21	2:J:83:ARG:CZ	2.48	0.44
1:I:48:VAL:O	1:I:48:VAL:CG1	2.65	0.44
1:I:135:PRO:HG2	1:I:144:VAL:HG12	2.00	0.44
2:M:143:ALA:HB2	2:P:143:ALA:HB1	2.00	0.44
2:P:84:ALA:O	2:P:87:VAL:HG12	2.18	0.44
1:B:85:LEU:HD21	2:D:83:ARG:CZ	2.47	0.44
1:C:4:SER:C	1:C:6:ALA:H	2.21	0.44
2:D:179:ASP:OD2	2:D:239:ALA:HA	2.17	0.44
1:E:183:LYS:HG3	1:E:184:GLN:HG3	1.99	0.44
1:H:221:LEU:HD13	1:H:221:LEU:H	1.79	0.44
1:H:244:GLN:HG3	1:H:266:ILE:HG22	2.00	0.44
2:G:248:VAL:HG12	2:G:265:VAL:HG23	2.00	0.44
1:I:78:ALA:HB1	1:I:82:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:226:LEU:HD23	2:J:227:PRO:HD2	2.00	0.44
2:M:271:THR:OG1	2:M:273:VAL:HG23	2.17	0.44
1:B:104:SER:HA	1:B:149:MET:HG3	1.99	0.44
1:B:109:GLN:NE2	2:D:108:GLU:OE2	2.43	0.44
1:B:126:VAL:HG13	1:B:145:VAL:O	2.18	0.44
1:B:154:LEU:HD21	2:A:181:PHE:CZ	2.53	0.44
1:C:163:VAL:O	1:C:163:VAL:CG1	2.66	0.44
2:G:138:ALA:HB1	2:J:124:GLY:CA	2.46	0.44
1:I:114:LEU:HG	1:I:118:LEU:HD11	2.00	0.44
1:O:154:LEU:HD21	2:P:181:PHE:CE1	2.52	0.44
1:B:133:ALA:O	1:B:137:SER:HB3	2.18	0.43
1:B:219:LYS:O	1:B:221:LEU:CD2	2.66	0.43
1:C:9:GLU:O	1:C:9:GLU:HG2	2.17	0.43
1:H:241:ARG:HE	1:H:269:ALA:HB3	1.83	0.43
1:I:222:HIS:O	1:I:224:SER:N	2.51	0.43
1:K:263:VAL:O	1:K:263:VAL:HG22	2.18	0.43
2:L:107:SER:O	2:L:111:GLN:HG2	2.18	0.43
2:M:83:ARG:NE	2:M:108:GLU:OE1	2.31	0.43
1:Q:59:LEU:CD2	1:Q:254:LEU:HD22	2.48	0.43
1:B:208:ILE:HG21	1:B:211:ILE:HB	2.00	0.43
2:A:166:PRO:O	2:A:169:ARG:NH1	2.50	0.43
1:C:8:LEU:HD12	1:C:8:LEU:HA	1.82	0.43
1:H:71:LYS:HB3	1:H:136:LEU:HD23	1.99	0.43
1:I:213:VAL:HA	1:I:216:MET:CG	2.47	0.43
1:I:228:PHE:CG	1:I:229:PRO:HD3	2.53	0.43
2:J:175:PHE:HA	2:J:186:LEU:HD22	1.98	0.43
1:K:222:HIS:HB3	1:K:228:PHE:CG	2.52	0.43
1:N:67:ARG:NH1	1:N:121:HIS:O	2.49	0.43
1:B:148:GLY:O	1:B:172:GLY:HA3	2.18	0.43
1:B:228:PHE:CD2	1:B:229:PRO:HD3	2.53	0.43
1:C:226:LEU:HB3	1:C:230:VAL:HG11	2.01	0.43
1:C:246:VAL:HG13	1:C:253:ASN:HB3	2.00	0.43
2:F:43:VAL:CG1	2:F:186:LEU:HD13	2.48	0.43
1:H:43:ILE:HD13	1:H:188:VAL:HG21	2.00	0.43
2:J:252:VAL:HG11	2:J:255:ARG:CZ	2.48	0.43
2:J:252:VAL:O	2:J:252:VAL:CG1	2.65	0.43
1:O:46:GLN:HB2	1:O:79:GLY:HA2	2.00	0.43
1:O:195:TYR:HB3	1:O:205:ALA:HB1	2.00	0.43
1:O:203:LYS:O	1:O:204:ASP:OD1	2.36	0.43
2:A:159:GLU:OE2	2:A:168:HIS:ND1	2.43	0.43
1:C:95:PRO:HG2	1:C:98:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:GLY:O	1:E:172:GLY:HA3	2.19	0.43
1:E:185:MET:HB3	1:E:243:VAL:HG12	2.01	0.43
2:G:88:PHE:CZ	2:G:165:ILE:HD11	2.53	0.43
1:I:136:LEU:HD12	1:I:136:LEU:H	1.83	0.43
2:P:88:PHE:CD2	2:P:165:ILE:HD12	2.54	0.43
1:Q:11:LEU:HD22	1:Q:15:ARG:HD2	2.00	0.43
1:Q:17:LEU:O	1:Q:23:GLN:NE2	2.43	0.43
1:H:32:PHE:CE2	1:H:34:ILE:HD13	2.53	0.43
1:H:192:ASP:O	1:H:207:PHE:HZ	2.02	0.43
1:H:211:ILE:HD12	1:H:215:GLU:CD	2.39	0.43
1:I:192:ASP:HA	1:I:247:ASN:HB2	2.01	0.43
1:K:213:VAL:HG21	1:K:235:GLN:CG	2.49	0.43
2:L:33:ARG:HA	2:L:240:ARG:HH21	1.84	0.43
2:L:52:ASP:OD1	2:L:52:ASP:N	2.51	0.43
2:L:214:THR:HG22	2:L:215:SER:N	2.34	0.43
1:O:64:VAL:O	1:O:67:ARG:HG2	2.19	0.43
1:O:185:MET:HB3	1:O:243:VAL:HG22	2.00	0.43
1:O:247:ASN:ND2	1:O:249:LEU:HB2	2.33	0.43
2:P:246:GLN:HG2	2:P:248:VAL:HG13	2.00	0.43
2:R:139:ILE:HG22	2:R:140:HIS:N	2.32	0.43
1:H:16:SER:HB3	2:G:225:PRO:HB3	1.99	0.43
1:K:138:LEU:HB2	1:K:141:VAL:CG1	2.48	0.43
2:R:206:GLY:O	2:R:207:GLN:HG2	2.18	0.43
1:B:53:ARG:HA	1:B:57:TYR:CD1	2.54	0.43
2:F:246:GLN:HB2	2:F:268:LEU:HD23	1.99	0.43
1:I:51:ARG:HD2	1:I:55:ALA:HB2	2.01	0.43
1:N:13:MET:HG2	2:M:82:VAL:CG2	2.49	0.43
1:B:235:GLN:HA	1:B:269:ALA:HB1	2.01	0.43
2:A:246:GLN:HG2	2:A:248:VAL:HG13	2.01	0.43
1:C:211:ILE:O	1:C:267:ILE:HA	2.19	0.43
1:C:250:VAL:HB	1:C:253:ASN:ND2	2.33	0.43
1:E:174:PHE:CD2	1:E:230:VAL:HG13	2.54	0.43
1:H:155:TRP:O	2:G:176:LEU:HD13	2.19	0.43
1:I:228:PHE:CD2	1:I:229:PRO:HD3	2.54	0.43
1:K:140:GLU:HG2	1:K:141:VAL:N	2.34	0.43
1:N:86:TYR:OH	1:N:103:GLY:HA3	2.18	0.43
1:O:213:VAL:HG21	1:O:235:GLN:OE1	2.18	0.43
2:R:198:ALA:O	2:R:208:ALA:CB	2.67	0.43
1:B:240:VAL:O	1:B:240:VAL:HG12	2.18	0.43
1:C:46:GLN:HA	1:C:50:ASP:OD2	2.19	0.43
2:F:124:GLY:O	2:F:144:THR:OG1	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:252:VAL:HB	2:F:255:ARG:HH11	1.83	0.43
1:H:64:VAL:O	1:H:68:LYS:HE3	2.19	0.43
1:H:125:VAL:CG2	1:I:131:LEU:HB3	2.48	0.43
1:N:152:TYR:HB3	1:N:156:MET:HA	2.01	0.43
1:B:154:LEU:HD21	2:A:181:PHE:CE1	2.54	0.43
1:E:67:ARG:NH1	1:E:121:HIS:O	2.51	0.43
1:H:211:ILE:HD13	1:H:211:ILE:HA	1.94	0.43
2:G:144:THR:HG23	2:G:146:ALA:H	1.84	0.43
1:I:85:LEU:CD2	2:L:83:ARG:CZ	2.96	0.43
2:J:240:ARG:C	2:J:273:VAL:HG13	2.39	0.43
2:L:132:THR:O	2:L:136:GLN:N	2.51	0.43
1:N:134:VAL:CG2	1:Q:124:PRO:HG3	2.49	0.43
1:Q:14:GLN:HG3	2:R:203:PRO:HD3	2.01	0.43
1:Q:138:LEU:CD1	1:Q:138:LEU:H	2.32	0.43
1:Q:203:LYS:HG3	1:Q:204:ASP:CG	2.40	0.43
1:C:228:PHE:N	1:C:229:PRO:HD2	2.34	0.42
1:H:57:TYR:HE1	2:J:94:LEU:HD23	1.84	0.42
2:L:110:GLY:O	2:L:114:HIS:ND1	2.48	0.42
2:R:264:HIS:CD2	2:R:266:GLY:O	2.71	0.42
1:K:185:MET:CG	1:K:243:VAL:HG12	2.49	0.42
2:M:83:ARG:O	2:M:87:VAL:HG23	2.20	0.42
2:R:198:ALA:O	2:R:208:ALA:HB1	2.19	0.42
2:A:43:VAL:O	2:A:186:LEU:HA	2.19	0.42
2:D:139:ILE:HG13	2:F:126:SER:HB2	2.02	0.42
2:F:177:LEU:HG	2:F:181:PHE:CE2	2.54	0.42
1:H:43:ILE:HG12	1:H:75:GLY:O	2.19	0.42
1:H:158:PRO:O	2:G:238:THR:OG1	2.36	0.42
1:I:44:GLY:HA3	1:I:189:LYS:HE3	2.02	0.42
1:I:220:GLY:O	1:I:221:LEU:C	2.57	0.42
1:I:243:VAL:CG1	1:I:244:GLN:N	2.81	0.42
1:K:175:LEU:O	1:K:179:GLN:HG2	2.19	0.42
1:N:51:ARG:HB2	1:N:55:ALA:HB3	2.01	0.42
2:M:232:LEU:HA	2:M:235:VAL:HG22	2.01	0.42
2:P:128:VAL:HG23	2:P:133:VAL:HG22	2.02	0.42
1:H:243:VAL:HG12	1:H:244:GLN:N	2.34	0.42
1:I:97:GLY:HA2	1:I:156:MET:HB3	2.00	0.42
1:K:3:ASN:HB3	1:K:7:GLU:OE1	2.19	0.42
1:K:8:LEU:C	1:K:11:LEU:H	2.22	0.42
1:K:33:ARG:HD2	1:K:36:PRO:HB3	2.01	0.42
1:K:213:VAL:CG2	1:K:214:ASP:N	2.83	0.42
2:R:232:LEU:HA	2:R:235:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:O	1:B:222:HIS:C	2.58	0.42
1:C:77:GLY:O	1:C:110:ASN:ND2	2.44	0.42
2:D:36:ARG:NH2	2:D:275:PRO:HG2	2.34	0.42
1:I:140:GLU:OE2	1:K:139:ALA:N	2.47	0.42
2:J:107:SER:O	2:J:111:GLN:HG2	2.19	0.42
2:J:244:ARG:HA	2:J:269:ILE:O	2.19	0.42
1:N:100:ALA:HB3	1:N:153:LYS:O	2.19	0.42
2:M:130:HIS:NE2	2:M:152:PHE:O	2.49	0.42
1:O:23:GLN:NE2	2:P:163:SER:OG	2.47	0.42
1:C:190:ASP:CB	1:C:249:LEU:HD21	2.50	0.42
1:E:132:SER:HB3	1:E:135:PRO:CD	2.50	0.42
1:E:225:ILE:HG12	1:E:245:VAL:HG11	2.00	0.42
1:H:55:ALA:HA	1:H:249:LEU:CD1	2.50	0.42
2:G:133:VAL:HA	2:G:137:LEU:HD11	2.01	0.42
1:I:229:PRO:O	1:I:233:LEU:N	2.45	0.42
1:I:229:PRO:O	1:I:233:LEU:HG	2.20	0.42
2:M:96:LEU:HD13	1:Q:116:GLN:OE1	2.19	0.42
2:P:144:THR:HG23	2:P:145:ARG:N	2.35	0.42
2:A:143:ALA:HB1	2:F:143:ALA:HB2	2.01	0.42
1:H:237:ALA:O	1:H:241:ARG:HD2	2.19	0.42
2:G:43:VAL:HG13	2:G:186:LEU:HA	2.02	0.42
2:G:165:ILE:HD12	2:G:166:PRO:CD	2.50	0.42
1:I:84:HIS:HE1	2:L:52:ASP:OD2	2.01	0.42
1:K:78:ALA:N	1:K:169:THR:HG21	2.35	0.42
2:L:61:LEU:HD13	2:L:250:GLY:O	2.19	0.42
2:P:271:THR:OG1	2:P:273:VAL:HG23	2.20	0.42
1:Q:170:ASP:HB2	1:Q:227:GLU:CD	2.40	0.42
1:B:136:LEU:O	1:B:142:ASN:HA	2.20	0.42
2:A:175:PHE:HA	2:A:186:LEU:HD22	2.01	0.42
1:H:48:VAL:HG11	1:H:59:LEU:CD1	2.49	0.42
1:H:81:ARG:NH2	1:H:106:VAL:HG13	2.35	0.42
1:H:149:MET:SD	1:H:150:PRO:HD2	2.60	0.42
1:I:43:ILE:HG22	1:I:48:VAL:HB	2.02	0.42
1:I:183:LYS:HG3	1:I:184:GLN:N	2.35	0.42
1:N:176:LEU:HD12	1:N:176:LEU:HA	1.94	0.42
1:O:122:GLY:CA	1:Q:137:SER:OG	2.68	0.42
2:D:209:ARG:O	2:D:211:LEU:HD12	2.20	0.42
2:F:82:VAL:HA	2:F:85:ARG:HG2	2.02	0.42
1:H:73:LEU:HD11	1:H:136:LEU:HD21	2.02	0.42
2:G:83:ARG:CZ	1:K:85:LEU:HG	2.50	0.42
1:K:78:ALA:HB1	1:K:82:ALA:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:98:VAL:O	1:K:102:LEU:HD13	2.20	0.42
1:N:138:LEU:HD12	1:N:141:VAL:HB	2.02	0.42
1:O:53:ARG:HA	2:R:94:LEU:HD23	2.02	0.42
1:O:187:PHE:HD1	1:O:243:VAL:CG1	2.33	0.42
2:P:193:ASP:HA	2:P:249:ASN:HB2	2.01	0.42
2:R:177:LEU:HG	2:R:181:PHE:CE2	2.55	0.42
2:A:53:ARG:NH1	2:A:251:LEU:HD13	2.35	0.42
2:A:77:LEU:HD11	2:A:177:LEU:HD23	2.02	0.42
1:E:100:ALA:HB3	1:E:153:LYS:O	2.20	0.42
2:F:127:TYR:CE1	2:F:149:GLY:HA2	2.55	0.42
1:H:219:LYS:HA	1:H:219:LYS:CD	2.49	0.42
1:H:219:LYS:C	1:H:221:LEU:N	2.73	0.42
1:I:22:LEU:CD2	2:J:165:ILE:CD1	2.98	0.42
1:K:8:LEU:N	1:K:8:LEU:CD1	2.79	0.42
1:K:123:ILE:CD1	1:K:143:ALA:HB3	2.50	0.42
1:N:77:GLY:HA2	1:N:169:THR:HG21	2.01	0.42
1:O:148:GLY:O	1:O:172:GLY:HA3	2.20	0.42
1:Q:101:GLN:HB2	1:Q:153:LYS:HD3	2.00	0.42
1:Q:211:ILE:O	1:Q:267:ILE:HA	2.20	0.42
2:R:271:THR:OG1	2:R:273:VAL:CG2	2.68	0.42
1:C:18:THR:HG22	2:D:230:ARG:HG3	2.01	0.41
1:H:47:SER:OG	1:H:189:LYS:HD2	2.20	0.41
1:K:73:LEU:HD11	1:K:136:LEU:HD21	2.02	0.41
1:K:217:LYS:HE2	1:K:232:ASP:OD1	2.20	0.41
1:N:4:SER:OG	1:N:5:THR:N	2.53	0.41
2:M:87:VAL:HG21	1:Q:109:GLN:HE22	1.85	0.41
2:R:248:VAL:CG1	2:R:265:VAL:HG23	2.49	0.41
1:C:99:LEU:CD2	1:C:163:VAL:HG12	2.49	0.41
1:E:30:ALA:O	2:F:95:GLY:HA2	2.20	0.41
1:H:88:ILE:CD1	2:J:52:ASP:HA	2.50	0.41
1:H:102:LEU:HD21	2:J:115:ILE:HG13	2.02	0.41
1:H:155:TRP:CE3	2:G:154:PRO:HD2	2.55	0.41
2:G:99:GLY:O	2:G:156:HIS:O	2.37	0.41
2:J:103:PRO:HD3	2:J:156:HIS:HB3	2.02	0.41
2:A:248:VAL:HG11	2:A:259:ALA:HB2	2.02	0.41
1:C:16:SER:HB3	2:D:225:PRO:CB	2.50	0.41
1:C:185:MET:HB3	1:C:243:VAL:HG12	2.02	0.41
2:F:130:HIS:N	2:F:131:PRO:HD2	2.35	0.41
2:G:100:SER:O	2:G:104:LEU:HG	2.19	0.41
2:G:252:VAL:HG21	2:G:255:ARG:HD2	2.02	0.41
2:J:152:PHE:CE1	2:J:170:ALA:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:194:LEU:C	1:K:195:TYR:HD1	2.23	0.41
2:L:273:VAL:CG1	2:L:274:ARG:N	2.83	0.41
2:M:130:HIS:N	2:M:131:PRO:HD2	2.36	0.41
1:O:131:LEU:C	1:O:131:LEU:HD23	2.41	0.41
1:O:228:PHE:N	1:O:229:PRO:CD	2.84	0.41
2:P:199:ASP:OD1	4:P:301:ATP:N9	2.53	0.41
2:A:193:ASP:HB2	2:A:196:TYR:OH	2.20	0.41
1:C:250:VAL:HB	1:C:253:ASN:HD21	1.85	0.41
1:E:9:GLU:O	1:E:9:GLU:HG2	2.21	0.41
1:H:226:LEU:CD1	1:H:231:LEU:CD2	2.97	0.41
2:J:160:PHE:N	2:J:160:PHE:CD1	2.88	0.41
1:K:74:ILE:HD12	1:K:144:VAL:O	2.20	0.41
2:L:75:LEU:HD21	2:L:77:LEU:HD21	2.02	0.41
2:L:219:LEU:CB	2:L:233:LEU:HD21	2.50	0.41
2:F:80:ALA:HB2	2:F:152:PHE:CE1	2.55	0.41
1:H:57:TYR:CE1	2:J:94:LEU:HD23	2.56	0.41
2:G:205:ARG:O	2:G:205:ARG:HG2	2.20	0.41
1:I:213:VAL:HG23	1:I:214:ASP:N	2.36	0.41
2:J:42:GLN:NE2	2:J:184:ALA:HB3	2.34	0.41
1:O:191:GLU:HG3	1:O:199:PRO:HG2	2.01	0.41
1:Q:10:GLU:OE1	1:Q:13:MET:CE	2.68	0.41
1:Q:138:LEU:HB2	1:Q:141:VAL:HB	2.02	0.41
1:Q:213:VAL:HG23	1:Q:214:ASP:N	2.35	0.41
1:Q:246:VAL:CG1	1:Q:253:ASN:HB3	2.50	0.41
2:A:55:ALA:HB1	2:A:59:LEU:CD1	2.50	0.41
1:C:8:LEU:HD22	1:C:26:ALA:N	2.35	0.41
2:D:130:HIS:N	2:D:131:PRO:HD2	2.35	0.41
1:H:92:LEU:HD21	2:J:58:ILE:HD13	2.03	0.41
1:H:151:PRO:HD3	2:G:158:HIS:CG	2.56	0.41
2:G:44:VAL:HG12	2:G:45:LYS:N	2.35	0.41
2:G:69:LEU:N	2:G:70:PRO:HD2	2.35	0.41
2:G:88:PHE:CD1	2:G:165:ILE:HD11	2.55	0.41
2:G:89:SER:O	2:G:93:ASP:N	2.43	0.41
2:G:236:MET:CE	2:G:269:ILE:HG21	2.50	0.41
1:I:228:PHE:N	1:I:229:PRO:HD2	2.35	0.41
2:J:53:ARG:HA	2:J:53:ARG:HE	1.82	0.41
2:J:71:GLU:HG2	2:J:72:HIS:CD2	2.55	0.41
2:J:214:THR:O	2:J:269:ILE:HA	2.20	0.41
1:K:62:GLU:OE2	1:K:254:LEU:HB3	2.20	0.41
2:L:42:GLN:HB2	2:L:74:LEU:HD23	2.01	0.41
1:O:125:VAL:HG13	1:O:145:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:217:LYS:HE2	1:O:231:LEU:HB3	2.02	0.41
1:Q:80:THR:O	1:Q:83:ARG:HB2	2.20	0.41
1:Q:178:GLU:OE1	1:Q:237:ALA:HB1	2.20	0.41
1:B:13:MET:O	2:A:49:ARG:NH2	2.53	0.41
1:H:248:GLY:O	1:H:249:LEU:HB2	2.21	0.41
2:G:120:LEU:HD22	2:G:125:VAL:CG2	2.51	0.41
2:G:215:SER:HB2	2:G:270:ARG:NH2	2.36	0.41
1:K:237:ALA:HA	2:L:161:PRO:CB	2.48	0.41
1:N:131:LEU:HD22	1:Q:125:VAL:HB	2.03	0.41
1:O:43:ILE:HG22	1:O:49:ILE:HG13	2.02	0.41
1:E:67:ARG:HD3	1:E:123:ILE:HD11	2.03	0.41
1:E:132:SER:HB3	1:E:135:PRO:HD2	2.02	0.41
1:E:225:ILE:CG2	1:E:226:LEU:N	2.83	0.41
1:I:7:GLU:O	1:I:11:LEU:HD13	2.21	0.41
1:I:19:ASP:O	1:I:23:GLN:HG2	2.20	0.41
1:K:61:ASP:O	1:K:64:VAL:CG2	2.68	0.41
1:N:126:VAL:HG13	1:N:144:VAL:CG2	2.51	0.41
1:O:17:LEU:HD23	1:O:22:LEU:CD1	2.50	0.41
1:O:81:ARG:NH2	1:O:110:ASN:OD1	2.46	0.41
1:O:247:ASN:CG	1:O:249:LEU:HB2	2.41	0.41
2:R:79:GLY:O	2:R:109:ALA:HA	2.20	0.41
1:B:26:ALA:O	2:A:164:ARG:HG3	2.21	0.41
1:B:247:ASN:OD1	1:B:249:LEU:HB2	2.21	0.41
4:A:301:ATP:N3	4:A:301:ATP:C2'	2.83	0.41
1:C:152:TYR:HB3	1:C:156:MET:HA	2.02	0.41
2:D:107:SER:O	2:D:111:GLN:HG2	2.21	0.41
1:E:108:ASP:OD1	1:E:147:SER:OG	2.34	0.41
1:E:195:TYR:CD1	1:E:207:PHE:N	2.89	0.41
1:E:213:VAL:O	1:E:216:MET:N	2.52	0.41
2:F:33:ARG:HH22	2:F:36:ARG:NH2	2.19	0.41
2:F:193:ASP:OD1	2:F:249:ASN:ND2	2.49	0.41
1:H:56:VAL:HG13	1:H:57:TYR:N	2.36	0.41
1:H:76:THR:HG21	1:H:111:ALA:N	2.36	0.41
1:H:151:PRO:CD	2:G:158:HIS:CD2	2.99	0.41
2:G:66:ARG:HG2	2:G:123:GLU:HG3	2.02	0.41
2:G:204:ASP:O	2:G:207:GLN:N	2.45	0.41
1:I:78:ALA:O	1:I:106:VAL:HG12	2.21	0.41
1:I:85:LEU:HD13	1:I:102:LEU:HB3	2.01	0.41
1:I:102:LEU:O	1:I:105:SER:OG	2.35	0.41
1:I:118:LEU:CB	1:I:123:ILE:CG2	2.95	0.41
1:I:122:GLY:HA3	1:K:137:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:134:VAL:N	1:I:135:PRO:CD	2.84	0.41
1:I:216:MET:CE	1:I:221:LEU:CD1	2.85	0.41
2:J:160:PHE:HB2	2:J:167:PRO:HG2	2.01	0.41
1:K:140:GLU:HG2	1:K:141:VAL:H	1.85	0.41
1:K:154:LEU:HD22	2:L:177:LEU:CD1	2.47	0.41
2:L:173:GLY:HA2	2:L:176:LEU:HD12	2.03	0.41
1:N:52:GLY:O	1:N:56:VAL:HG23	2.21	0.41
1:N:148:GLY:O	1:N:172:GLY:HA3	2.20	0.41
1:N:223:ASP:OD1	1:N:227:GLU:HA	2.21	0.41
2:M:59:LEU:HB2	2:M:60:PRO:HD3	2.03	0.41
1:O:17:LEU:HA	1:O:22:LEU:HD13	2.02	0.41
1:Q:191:GLU:HG3	1:Q:199:PRO:HG2	2.01	0.41
2:R:133:VAL:HG12	2:R:177:LEU:HD21	2.01	0.41
2:R:197:THR:OG1	2:R:208:ALA:HA	2.21	0.41
1:C:224:SER:H	1:C:224:SER:HG	1.59	0.41
2:D:197:THR:HB	2:D:211:LEU:HD11	2.02	0.41
2:F:43:VAL:HG12	2:F:186:LEU:CD1	2.51	0.41
2:G:92:LEU:CD2	2:G:164:ARG:HD2	2.50	0.41
1:K:93:GLY:HA3	2:L:35:ILE:HG23	2.03	0.41
1:O:141:VAL:HG12	1:O:143:ALA:H	1.85	0.41
1:O:221:LEU:CD2	1:O:224:SER:OG	2.69	0.41
1:B:8:LEU:C	1:B:10:GLU:N	2.73	0.40
2:A:83:ARG:CZ	1:E:85:LEU:HD21	2.51	0.40
2:D:215:SER:HB2	2:D:270:ARG:NH1	2.35	0.40
1:E:152:TYR:O	1:E:155:TRP:N	2.54	0.40
1:E:172:GLY:HA2	2:F:158:HIS:CD2	2.56	0.40
1:H:116:GLN:O	1:I:34:ILE:HG23	2.21	0.40
2:G:179:ASP:OD2	2:G:239:ALA:HB1	2.22	0.40
2:L:265:VAL:HG23	2:L:266:GLY:H	1.85	0.40
1:N:134:VAL:HG12	1:N:138:LEU:HD21	2.03	0.40
1:O:59:LEU:O	1:O:63:ILE:HG13	2.21	0.40
2:P:201:ASN:OD1	4:P:301:ATP:O2'	2.34	0.40
1:Q:5:THR:CG2	2:R:93:ASP:OD1	2.68	0.40
1:Q:8:LEU:O	1:Q:12:LEU:HG	2.21	0.40
1:B:81:ARG:NE	2:D:87:VAL:HG22	2.37	0.40
1:E:64:VAL:HG21	1:E:121:HIS:CE1	2.57	0.40
1:H:108:ASP:OD1	1:H:147:SER:CB	2.68	0.40
2:G:45:LYS:HD2	2:G:188:ILE:HD13	2.04	0.40
2:G:47:GLY:O	2:G:50:VAL:CG2	2.70	0.40
2:G:197:THR:HG23	2:G:211:LEU:HD11	2.02	0.40
1:I:179:GLN:OE1	2:J:97:PRO:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:208:ILE:O	1:I:208:ILE:CG2	2.69	0.40
2:L:43:VAL:HG12	2:L:186:LEU:CD1	2.51	0.40
2:L:96:LEU:HB2	2:L:101:LEU:HD21	2.02	0.40
2:L:199:ASP:H	2:L:225:PRO:HG2	1.86	0.40
1:N:7:GLU:CD	1:N:11:LEU:HD12	2.42	0.40
1:O:152:TYR:O	1:O:155:TRP:N	2.54	0.40
1:O:196:THR:HG22	1:O:208:ILE:HD11	2.02	0.40
1:O:225:ILE:HG23	1:O:226:LEU:HG	2.04	0.40
2:P:199:ASP:HB2	2:P:225:PRO:CG	2.51	0.40
1:Q:221:LEU:O	1:Q:222:HIS:C	2.60	0.40
1:E:179:GLN:HG3	2:F:157:HIS:O	2.21	0.40
1:H:19:ASP:OD1	1:H:20:PRO:HD2	2.21	0.40
1:H:211:ILE:HD12	1:H:215:GLU:OE1	2.20	0.40
1:H:213:VAL:HG22	1:H:269:ALA:O	2.21	0.40
2:G:130:HIS:N	2:G:131:PRO:HD2	2.36	0.40
2:G:223:GLU:HA	2:G:230:ARG:NH2	2.37	0.40
2:G:256:LEU:HD12	2:G:256:LEU:HA	1.92	0.40
1:I:31:ASP:OD2	1:I:239:HIS:NE2	2.54	0.40
2:J:124:GLY:O	2:J:144:THR:OG1	2.31	0.40
1:K:178:GLU:HA	1:K:240:VAL:HG12	2.02	0.40
1:N:167:TYR:CE1	1:N:229:PRO:HB2	2.56	0.40
1:O:99:LEU:HD22	1:O:163:VAL:O	2.21	0.40
2:R:172:THR:OG1	2:R:232:LEU:N	2.54	0.40
1:B:141:VAL:O	1:B:142:ASN:C	2.56	0.40
1:C:105:SER:O	1:C:109:GLN:HG3	2.22	0.40
2:D:214:THR:HG23	2:D:269:ILE:HG12	2.04	0.40
1:E:12:LEU:HD23	1:E:22:LEU:HD11	2.03	0.40
1:E:22:LEU:HD21	2:F:165:ILE:CD1	2.52	0.40
1:H:244:GLN:NE2	1:H:263:VAL:O	2.54	0.40
2:G:88:PHE:CE1	2:G:165:ILE:HD11	2.57	0.40
2:G:103:PRO:CB	2:G:156:HIS:HB3	2.41	0.40
1:I:41:ILE:CA	1:I:185:MET:HE1	2.52	0.40
1:I:78:ALA:O	1:I:106:VAL:CG1	2.69	0.40
1:I:78:ALA:O	1:I:110:ASN:ND2	2.52	0.40
2:L:193:ASP:HA	2:L:249:ASN:HB2	2.03	0.40
1:N:67:ARG:HD2	1:N:141:VAL:O	2.21	0.40
1:N:192:ASP:O	1:N:264:GLY:HA2	2.22	0.40
1:C:247:ASN:HB3	1:C:253:ASN:ND2	2.36	0.40
1:E:176:LEU:HD12	1:E:176:LEU:HA	1.93	0.40
2:G:190:GLU:OE1	2:G:227:PRO:HB2	2.21	0.40
1:I:188:VAL:O	1:I:188:VAL:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:255:THR:HA	1:I:258:LEU:HD12	2.03	0.40
2:J:139:ILE:HG13	2:L:126:SER:HB2	2.04	0.40
1:N:23:GLN:OE1	2:M:163:SER:OG	2.38	0.40
1:Q:154:LEU:HD21	2:R:181:PHE:CE1	2.57	0.40
2:R:198:ALA:HB1	2:R:204:ASP:OD2	2.22	0.40

All (2) 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:B:200:LYS:NZ	1:O:204:ASP:OD2[2_354]	2.07	0.13
1:B:200:LYS:HZ1	1:O:204:ASP:OD2[2_354]	1.56	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	266/269 (99%)	260 (98%)	6 (2%)	0	100	100
1	C	266/269 (99%)	253 (95%)	13 (5%)	0	100	100
1	E	267/269 (99%)	263 (98%)	4 (2%)	0	100	100
1	H	266/269 (99%)	255 (96%)	10 (4%)	1 (0%)	34	66
1	I	266/269 (99%)	252 (95%)	14 (5%)	0	100	100
1	K	266/269 (99%)	255 (96%)	11 (4%)	0	100	100
1	N	266/269 (99%)	257 (97%)	9 (3%)	0	100	100
1	O	266/269 (99%)	260 (98%)	6 (2%)	0	100	100
1	Q	266/269 (99%)	261 (98%)	5 (2%)	0	100	100
2	A	242/275 (88%)	240 (99%)	2 (1%)	0	100	100
2	D	242/275 (88%)	239 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	242/275 (88%)	238 (98%)	4 (2%)	0	100	100
2	G	242/275 (88%)	241 (100%)	1 (0%)	0	100	100
2	J	242/275 (88%)	239 (99%)	3 (1%)	0	100	100
2	L	242/275 (88%)	238 (98%)	4 (2%)	0	100	100
2	M	242/275 (88%)	239 (99%)	3 (1%)	0	100	100
2	P	242/275 (88%)	241 (100%)	1 (0%)	0	100	100
2	R	242/275 (88%)	233 (96%)	9 (4%)	0	100	100
All	All	4573/4896 (93%)	4464 (98%)	108 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	220	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	B	205/205 (100%)	199 (97%)	6 (3%)	42	76
1	C	205/205 (100%)	190 (93%)	15 (7%)	14	38
1	E	206/205 (100%)	198 (96%)	8 (4%)	32	66
1	H	205/205 (100%)	188 (92%)	17 (8%)	11	32
1	I	205/205 (100%)	187 (91%)	18 (9%)	10	29
1	K	205/205 (100%)	189 (92%)	16 (8%)	12	35
1	N	205/205 (100%)	198 (97%)	7 (3%)	37	71
1	O	205/205 (100%)	194 (95%)	11 (5%)	22	53
1	Q	205/205 (100%)	200 (98%)	5 (2%)	49	81
2	A	187/215 (87%)	182 (97%)	5 (3%)	44	78
2	D	187/215 (87%)	183 (98%)	4 (2%)	53	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	187/215 (87%)	184 (98%)	3 (2%)	62	88
2	G	187/215 (87%)	177 (95%)	10 (5%)	22	54
2	J	187/215 (87%)	177 (95%)	10 (5%)	22	54
2	L	187/215 (87%)	178 (95%)	9 (5%)	25	58
2	M	187/215 (87%)	177 (95%)	10 (5%)	22	54
2	P	187/215 (87%)	183 (98%)	4 (2%)	53	84
2	R	187/215 (87%)	180 (96%)	7 (4%)	34	68
All	All	3529/3780 (93%)	3364 (95%)	165 (5%)	26	59

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	THR
1	B	73	LEU
1	B	132	SER
1	B	137	SER
1	B	141	VAL
1	B	153	LYS
2	A	139	ILE
2	A	142	SER
2	A	209	ARG
2	A	211	LEU
2	A	274	ARG
1	C	4	SER
1	C	8	LEU
1	C	11	LEU
1	C	15	ARG
1	C	47	SER
1	C	80	THR
1	C	105	SER
1	C	138	LEU
1	C	144	VAL
1	C	153	LYS
1	C	189	LYS
1	C	192	ASP
1	C	210	ARG
1	C	230	VAL
1	C	232	ASP
2	D	50	VAL
2	D	207	GLN

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Mol	Chain	Res	Type
2	D	214	THR
2	D	274	ARG
1	E	8	LEU
1	E	35	LEU
1	E	69	ASN
1	E	126	VAL
1	E	144	VAL
1	E	196	THR
1	E	200	LYS
1	E	255	THR
2	F	144	THR
2	F	214	THR
2	F	244	ARG
1	H	15	ARG
1	H	17	LEU
1	H	42	LYS
1	H	68	LYS
1	H	70	HIS
1	H	71	LYS
1	H	87	SER
1	H	118	LEU
1	H	131	LEU
1	H	134	VAL
1	H	138	LEU
1	H	140	GLU
1	H	141	VAL
1	H	219	LYS
1	H	221	LEU
1	H	223	ASP
1	H	247	ASN
2	G	33	ARG
2	G	111	GLN
2	G	120	LEU
2	G	144	THR
2	G	164	ARG
2	G	205	ARG
2	G	214	THR
2	G	226	LEU
2	G	238	THR
2	G	269	ILE
1	I	72	LEU
1	I	99	LEU

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Mol	Chain	Res	Type
1	I	105	SER
1	I	120	LYS
1	I	134	VAL
1	I	140	GLU
1	I	141	VAL
1	I	149	MET
1	I	161	GLU
1	I	168	ARG
1	I	180	PHE
1	I	204	ASP
1	I	207	PHE
1	I	214	ASP
1	I	222	HIS
1	I	226	LEU
1	I	238	GLN
1	I	268	THR
2	J	37	LEU
2	J	51	MET
2	J	77	LEU
2	J	85	ARG
2	J	107	SER
2	J	144	THR
2	J	204	ASP
2	J	251	LEU
2	J	252	VAL
2	J	270	ARG
1	K	4	SER
1	K	12	LEU
1	K	13	MET
1	K	67	ARG
1	K	85	LEU
1	K	105	SER
1	K	125	VAL
1	K	126	VAL
1	K	131	LEU
1	K	153	LYS
1	K	194	LEU
1	K	200	LYS
1	K	221	LEU
1	K	235	GLN
1	K	246	VAL
1	K	262	HIS

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Mol	Chain	Res	Type
2	L	41	LEU
2	L	52	ASP
2	L	59	LEU
2	L	139	ILE
2	L	176	LEU
2	L	192	VAL
2	L	204	ASP
2	L	209	ARG
2	L	274	ARG
1	N	3	ASN
1	N	120	LYS
1	N	149	MET
1	N	201	THR
1	N	210	ARG
1	N	222	HIS
1	N	224	SER
2	M	50	VAL
2	M	53	ARG
2	M	67	LYS
2	M	132	THR
2	M	147	VAL
2	M	209	ARG
2	M	217	THR
2	M	234	ASP
2	M	273	VAL
2	M	274	ARG
1	O	8	LEU
1	O	41	ILE
1	O	68	LYS
1	O	131	LEU
1	O	132	SER
1	O	137	SER
1	O	153	LYS
1	O	196	THR
1	O	200	LYS
1	O	223	ASP
1	O	228	PHE
2	P	87	VAL
2	P	144	THR
2	P	217	THR
2	P	274	ARG
1	Q	3	ASN

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Mol	Chain	Res	Type
1	Q	22	LEU
1	Q	41	ILE
1	Q	73	LEU
1	Q	255	THR
2	R	136	GLN
2	R	139	ILE
2	R	144	THR
2	R	209	ARG
2	R	217	THR
2	R	273	VAL
2	R	274	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	158	HIS
2	J	241	HIS
1	K	222	HIS
1	O	222	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\# Z > 2$
3	SO4	N	302	-	4,4,4	0.21	0	6,6,6	0.13	0
3	SO4	E	301	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	D	301	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	N	301	-	4,4,4	0.22	0	6,6,6	0.09	0
4	ATP	A	301	-	28,33,33	3.39	14 (50%)	34,52,52	3.24	5 (14%)
3	SO4	M	301	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	G	301	-	4,4,4	0.21	0	6,6,6	0.10	0
3	SO4	R	301	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	B	301	-	4,4,4	0.22	0	6,6,6	0.11	0
3	SO4	Q	301	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	F	301	-	4,4,4	0.21	0	6,6,6	0.12	0
4	ATP	P	301	-	28,33,33	3.36	14 (50%)	34,52,52	3.68	6 (17%)

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	P	301	-	-	0/18/38/38	0/3/3/3
4	ATP	A	301	-	-	8/18/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	ATP	C2'-C3'	-10.54	1.24	1.53
4	P	301	ATP	C2'-C3'	-9.92	1.26	1.53
4	A	301	ATP	PB-O3A	6.34	1.66	1.59
4	A	301	ATP	PA-O3A	6.30	1.66	1.59
4	P	301	ATP	PA-O3A	6.30	1.66	1.59
4	P	301	ATP	O4'-C1'	-6.14	1.32	1.40
4	P	301	ATP	PB-O3A	6.06	1.66	1.59
4	A	301	ATP	O4'-C1'	-5.59	1.33	1.40
4	A	301	ATP	PB-O3B	3.88	1.63	1.59
4	P	301	ATP	C5'-C4'	-3.74	1.40	1.51
4	A	301	ATP	C5'-C4'	-3.69	1.40	1.51
4	P	301	ATP	PB-O3B	3.63	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	301	ATP	O3'-C3'	3.30	1.51	1.43
4	P	301	ATP	C3'-C4'	3.24	1.61	1.53
4	P	301	ATP	C1'-N9	-3.16	1.42	1.49
4	A	301	ATP	O3'-C3'	3.08	1.50	1.43
4	P	301	ATP	O4'-C4'	3.06	1.51	1.45
4	A	301	ATP	O4'-C4'	2.96	1.51	1.45
4	A	301	ATP	PA-O5'	2.89	1.70	1.59
4	A	301	ATP	C3'-C4'	2.84	1.60	1.53
4	P	301	ATP	PA-O5'	2.83	1.70	1.59
4	A	301	ATP	C1'-N9	-2.72	1.43	1.49
4	P	301	ATP	C6-N6	2.70	1.43	1.34
4	A	301	ATP	C6-N6	2.70	1.43	1.34
4	A	301	ATP	O2'-C2'	2.56	1.49	1.43
4	P	301	ATP	O2'-C2'	2.47	1.49	1.43
4	A	301	ATP	C2-N3	2.05	1.35	1.32
4	P	301	ATP	C2-N3	2.01	1.35	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	301	ATP	C5-C6-N6	14.00	141.64	120.31
4	A	301	ATP	C5-C6-N6	13.50	140.88	120.31
4	P	301	ATP	N6-C6-N1	-9.52	97.98	118.33
4	A	301	ATP	N6-C6-N1	-9.21	98.65	118.33
4	P	301	ATP	C4'-O4'-C1'	-9.02	101.66	109.92
4	A	301	ATP	N3-C2-N1	-6.65	119.64	128.67
4	P	301	ATP	N3-C2-N1	-6.58	119.74	128.67
4	A	301	ATP	C1'-N9-C4	-4.60	118.56	126.64
4	P	301	ATP	C1'-N9-C4	-4.44	118.83	126.64
4	P	301	ATP	O4'-C1'-N9	2.89	112.58	108.75
4	A	301	ATP	C4'-O4'-C1'	-2.38	107.75	109.92

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	ATP	C5'-O5'-PA-O1A
4	A	301	ATP	C5'-O5'-PA-O2A
4	A	301	ATP	C5'-O5'-PA-O3A
4	A	301	ATP	O4'-C4'-C5'-O5'
4	A	301	ATP	C3'-C4'-C5'-O5'
4	A	301	ATP	PB-O3A-PA-O1A

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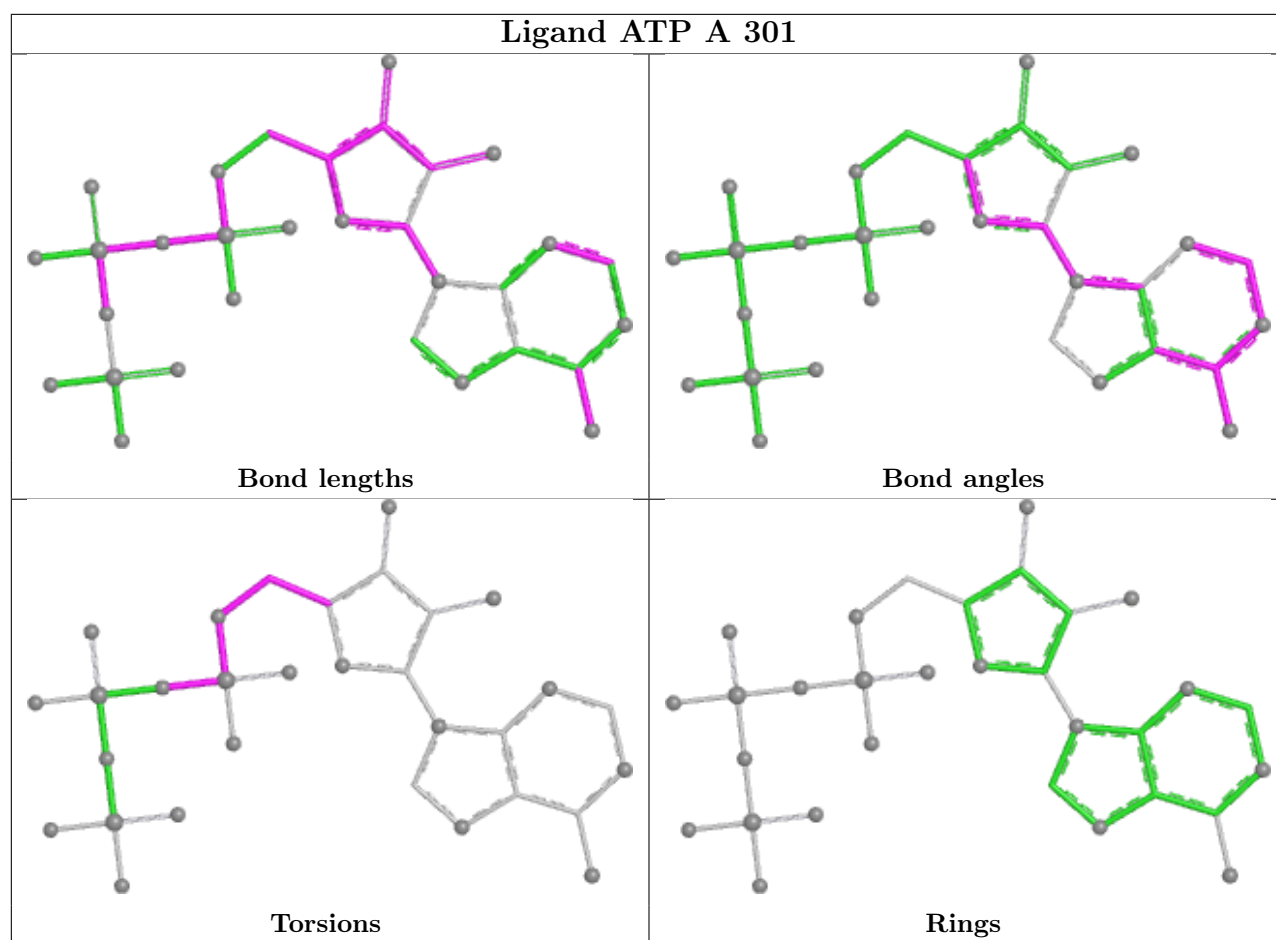
Mol	Chain	Res	Type	Atoms
4	A	301	ATP	C4'-C5'-O5'-PA
4	A	301	ATP	PB-O3A-PA-O2A

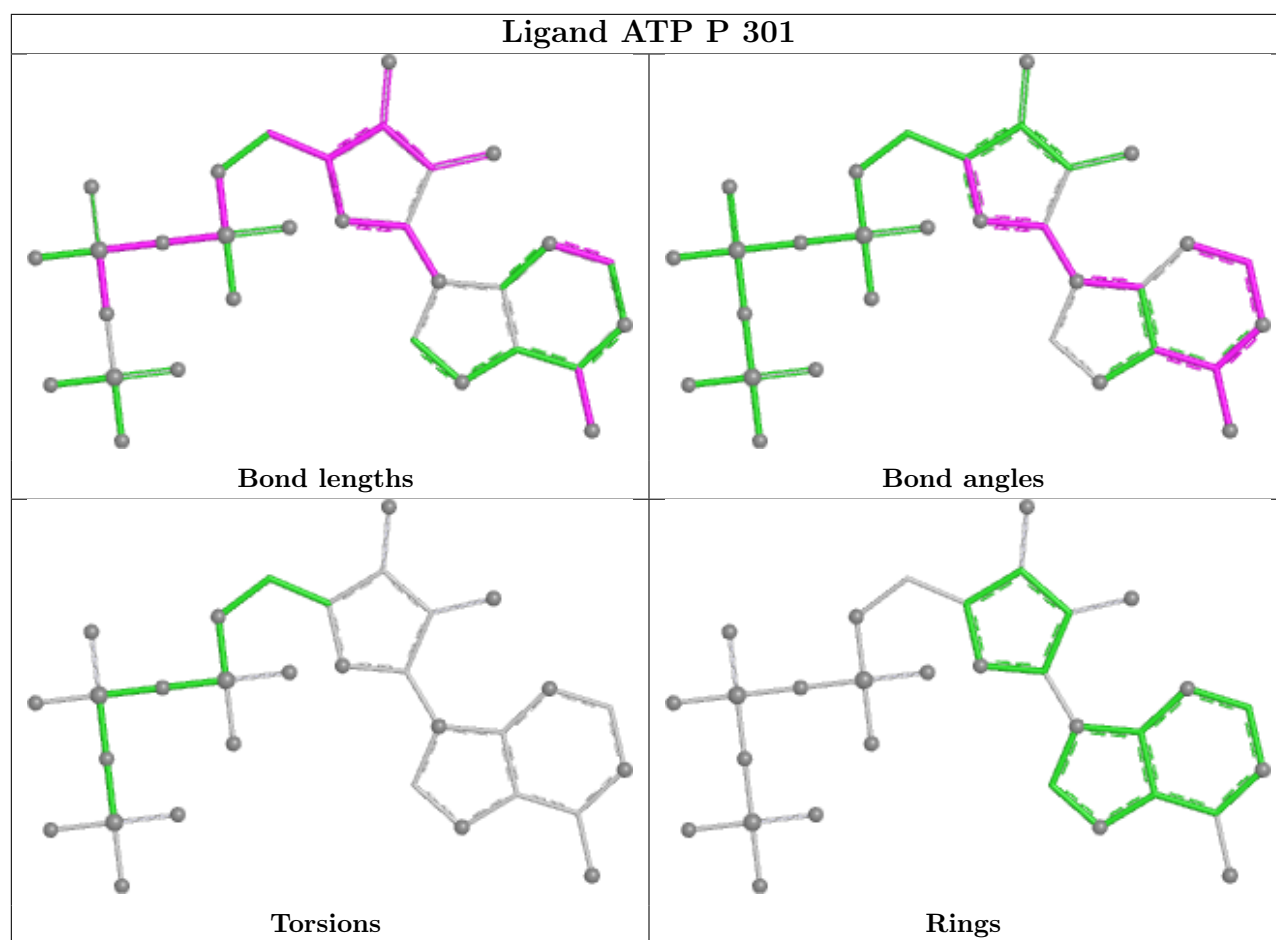
There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	302	SO4	1	0
3	E	301	SO4	2	0
4	A	301	ATP	3	0
3	B	301	SO4	1	0
4	P	301	ATP	5	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	268/269 (99%)	0.15	1 (0%) 92 91	20, 34, 58, 73	0
1	C	268/269 (99%)	0.38	9 (3%) 45 35	26, 44, 73, 88	0
1	E	268/269 (99%)	0.28	6 (2%) 62 52	22, 39, 67, 84	0
1	H	268/269 (99%)	1.17	52 (19%) 1 0	58, 81, 102, 108	0
1	I	268/269 (99%)	1.18	56 (20%) 1 0	60, 79, 96, 111	0
1	K	268/269 (99%)	0.95	47 (17%) 1 1	49, 72, 90, 99	0
1	N	268/269 (99%)	0.22	4 (1%) 73 68	17, 33, 61, 81	0
1	O	268/269 (99%)	0.19	6 (2%) 62 52	22, 39, 63, 78	0
1	Q	268/269 (99%)	0.23	7 (2%) 56 46	17, 33, 64, 83	0
2	A	244/275 (88%)	0.06	0 100 100	13, 22, 43, 55	0
2	D	244/275 (88%)	0.15	3 (1%) 79 73	14, 30, 63, 78	0
2	F	244/275 (88%)	0.14	1 (0%) 92 91	14, 29, 55, 74	0
2	G	244/275 (88%)	0.78	32 (13%) 3 2	48, 65, 83, 92	0
2	J	244/275 (88%)	0.92	34 (13%) 2 1	41, 65, 90, 99	0
2	L	244/275 (88%)	0.80	28 (11%) 4 2	43, 63, 83, 99	0
2	M	244/275 (88%)	0.09	0 100 100	13, 25, 49, 65	0
2	P	244/275 (88%)	0.11	1 (0%) 92 91	13, 24, 46, 62	0
2	R	244/275 (88%)	0.10	2 (0%) 86 81	13, 27, 53, 67	0
All	All	4608/4896 (94%)	0.44	289 (6%) 20 12	13, 42, 85, 111	0

All (289) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	5	THR	7.3
1	K	107	ALA	6.9
2	G	272	GLY	6.7

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Mol	Chain	Res	Type	RSRZ
1	I	163	VAL	6.7
1	K	199	PRO	6.5
1	H	27	ALA	6.2
1	I	112	ALA	6.1
1	H	28	ALA	5.8
2	G	98	VAL	5.4
1	I	22	LEU	5.2
2	J	220	ALA	5.2
1	I	24	ALA	5.1
1	K	267	ILE	5.1
2	J	196	TYR	5.1
2	L	208	ALA	5.1
1	H	254	LEU	5.0
1	I	230	VAL	5.0
2	G	246	GLN	5.0
1	K	60	VAL	4.9
1	I	100	ALA	4.9
2	J	161	PRO	4.8
1	K	139	ALA	4.7
2	L	91	GLY	4.7
1	I	225	ILE	4.7
2	J	197	THR	4.5
1	H	31	ASP	4.5
2	J	157	HIS	4.5
2	L	241	HIS	4.5
1	C	4	SER	4.4
1	I	202	SER	4.4
1	H	190	ASP	4.3
1	K	80	THR	4.3
2	L	273	VAL	4.3
1	K	196	THR	4.3
1	I	12	LEU	4.3
1	K	111	ALA	4.2
1	N	139	ALA	4.2
1	I	142	ASN	4.2
1	I	113	MET	4.2
1	H	125	VAL	4.1
1	I	186	ILE	4.1
1	H	18	THR	4.1
1	I	133	ALA	4.1
2	J	192	VAL	4.1
1	H	17	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	251	PRO	4.1
1	H	135	PRO	4.0
2	G	104	LEU	4.0
1	C	5	THR	4.0
1	K	138	LEU	3.9
1	H	140	GLU	3.9
2	R	272	GLY	3.9
1	I	4	SER	3.9
1	I	34	ILE	3.9
2	J	62	VAL	3.9
2	J	94	LEU	3.9
1	K	119	ALA	3.9
1	H	113	MET	3.8
2	J	193	ASP	3.8
1	K	177	ALA	3.8
1	N	199	PRO	3.7
2	G	219	LEU	3.7
1	I	180	PHE	3.7
2	J	147	VAL	3.7
1	H	12	LEU	3.7
1	H	16	SER	3.7
1	K	95	PRO	3.6
2	L	275	PRO	3.6
1	C	196	THR	3.6
2	J	61	LEU	3.6
2	D	275	PRO	3.6
2	L	266	GLY	3.5
1	I	40	VAL	3.5
1	I	30	ALA	3.5
2	G	229	ASP	3.5
1	H	199	PRO	3.5
1	K	6	ALA	3.5
2	G	240	ARG	3.5
1	K	8	LEU	3.4
1	H	88	ILE	3.4
1	I	125	VAL	3.4
1	C	8	LEU	3.4
1	Q	204	ASP	3.4
2	L	212	PRO	3.4
2	J	202	GLY	3.4
1	I	29	ALA	3.4
1	I	35	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	55	ALA	3.3
1	I	68	LYS	3.3
1	E	206	THR	3.3
2	L	215	SER	3.3
1	I	139	ALA	3.3
2	J	118	ALA	3.3
1	C	22	LEU	3.3
2	G	38	LEU	3.3
1	H	86	TYR	3.2
2	J	212	PRO	3.2
1	H	270	SER	3.2
2	D	198	ALA	3.2
2	G	40	TRP	3.2
1	I	13	MET	3.2
2	G	238	THR	3.2
1	H	24	ALA	3.2
1	I	211	ILE	3.2
2	G	178	ALA	3.2
2	G	239	ALA	3.2
1	I	248	GLY	3.1
2	L	228	VAL	3.1
1	H	236	SER	3.0
2	L	176	LEU	3.0
1	O	139	ALA	3.0
1	K	182	CYS	3.0
2	L	216	ALA	3.0
1	H	94	LEU	3.0
1	I	109	GLN	3.0
1	E	222	HIS	3.0
1	I	234	LEU	3.0
1	H	202	SER	3.0
1	H	48	VAL	3.0
1	K	251	PRO	2.9
2	G	185	GLY	2.9
1	I	260	GLY	2.9
2	J	195	ILE	2.9
1	K	133	ALA	2.9
2	J	206	GLY	2.9
1	H	133	ALA	2.9
1	I	127	GLY	2.9
1	I	116	GLN	2.9
1	H	93	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	201	THR	2.9
2	J	221	LYS	2.9
2	G	120	LEU	2.9
2	F	219	LEU	2.8
1	H	15	ARG	2.8
2	G	214	THR	2.8
2	J	227	PRO	2.8
1	I	223	ASP	2.8
1	H	261	GLU	2.8
1	H	173	CYS	2.8
1	H	96	ALA	2.8
2	G	274	ARG	2.7
1	N	209	PRO	2.7
1	K	159	ALA	2.7
2	L	172	THR	2.7
1	H	208	ILE	2.7
1	K	126	VAL	2.7
1	K	39	THR	2.7
2	D	272	GLY	2.7
2	L	78	THR	2.7
1	H	146	PHE	2.7
1	K	234	LEU	2.7
1	I	240	VAL	2.7
1	I	164	ILE	2.7
2	G	112	ASN	2.7
2	L	125	VAL	2.6
1	N	13	MET	2.6
1	Q	140	GLU	2.6
2	J	95	GLY	2.6
1	Q	14	GLN	2.6
2	G	183	ALA	2.6
2	J	106	ALA	2.6
2	J	268	LEU	2.6
1	Q	139	ALA	2.6
2	G	255	ARG	2.6
2	J	91	GLY	2.6
1	I	195	TYR	2.6
2	J	191	ASN	2.6
2	L	161	PRO	2.6
2	L	185	GLY	2.6
1	I	207	PHE	2.6
2	G	103	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	201	THR	2.5
1	H	5	THR	2.5
2	J	241	HIS	2.5
1	H	14	GLN	2.5
1	H	106	VAL	2.5
1	K	145	VAL	2.5
1	C	29	ALA	2.5
1	K	195	TYR	2.5
1	I	124	PRO	2.5
2	G	99	GLY	2.5
2	G	169	ARG	2.5
2	G	275	PRO	2.5
2	L	268	LEU	2.5
1	H	68	LYS	2.5
1	H	223	ASP	2.5
1	K	89	ALA	2.5
1	I	165	PRO	2.5
1	K	64	VAL	2.5
2	L	88	PHE	2.5
1	H	127	GLY	2.5
2	J	246	GLN	2.5
1	K	249	LEU	2.4
1	O	199	PRO	2.4
1	Q	223	ASP	2.4
1	I	25	ALA	2.4
2	P	216	ALA	2.4
2	G	267	THR	2.4
1	H	218	ALA	2.4
1	K	221	LEU	2.4
1	K	136	LEU	2.4
2	J	46	ILE	2.4
1	E	130	GLY	2.4
1	H	137	SER	2.4
1	K	118	LEU	2.4
1	H	95	PRO	2.4
2	L	148	VAL	2.4
1	K	237	ALA	2.4
1	H	130	GLY	2.4
1	K	246	VAL	2.4
1	K	186	ILE	2.4
1	I	206	THR	2.3
2	J	259	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	117	LEU	2.3
2	J	210	PHE	2.3
2	J	214	THR	2.3
1	I	193	GLY	2.3
2	L	221	LYS	2.3
2	J	143	ALA	2.3
2	L	37	LEU	2.3
1	I	16	SER	2.3
1	K	268	THR	2.3
1	O	196	THR	2.3
2	G	143	ALA	2.3
1	E	23	GLN	2.3
2	G	225	PRO	2.3
1	I	114	LEU	2.3
1	K	96	ALA	2.3
1	K	153	LYS	2.3
1	H	176	LEU	2.3
2	L	198	ALA	2.3
1	I	267	ILE	2.3
1	I	48	VAL	2.2
1	I	237	ALA	2.2
1	K	248	GLY	2.2
1	O	135	PRO	2.2
2	G	60	PRO	2.2
1	K	120	LYS	2.2
2	J	150	SER	2.2
1	K	160	ALA	2.2
2	G	37	LEU	2.2
1	H	9	GLU	2.2
1	H	67	ARG	2.2
1	H	238	GLN	2.2
2	G	273	VAL	2.2
2	J	126	SER	2.2
2	J	219	LEU	2.2
1	H	116	GLN	2.2
1	K	128	GLY	2.2
1	I	8	LEU	2.2
1	I	72	LEU	2.2
2	J	121	ALA	2.2
2	R	275	PRO	2.2
1	K	17	LEU	2.2
2	L	214	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	257	ALA	2.2
1	I	152	TYR	2.2
2	L	247	VAL	2.2
1	K	231	LEU	2.1
2	G	34	PRO	2.1
1	E	246	VAL	2.1
1	H	111	ALA	2.1
1	H	166	PRO	2.1
1	I	70	HIS	2.1
1	K	122	GLY	2.1
1	K	220	GLY	2.1
2	L	265	VAL	2.1
1	K	245	VAL	2.1
1	Q	250	VAL	2.1
2	L	99	GLY	2.1
2	L	128	VAL	2.1
1	E	203	LYS	2.1
1	H	39	THR	2.1
1	K	61	ASP	2.1
2	G	195	ILE	2.1
1	Q	135	PRO	2.1
1	O	217	LYS	2.1
1	O	141	VAL	2.1
1	I	90	ALA	2.1
1	C	21	GLN	2.1
1	I	51	ARG	2.1
1	B	131	LEU	2.1
2	G	170	ALA	2.1
1	H	230	VAL	2.1
1	C	259	ALA	2.0
1	I	162	GLY	2.0
1	K	198	ASN	2.0
1	H	112	ALA	2.0
1	H	200	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

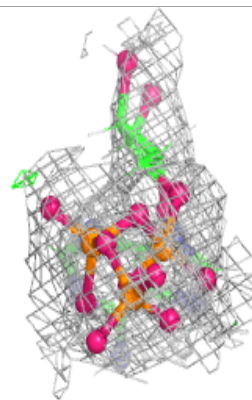
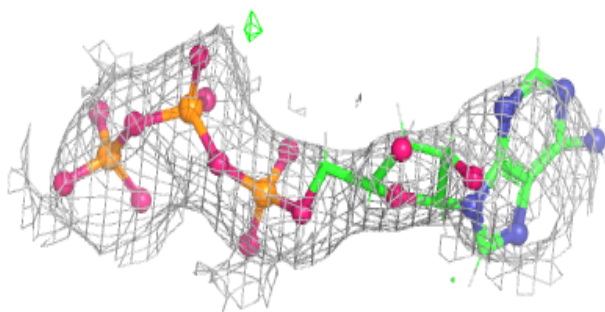
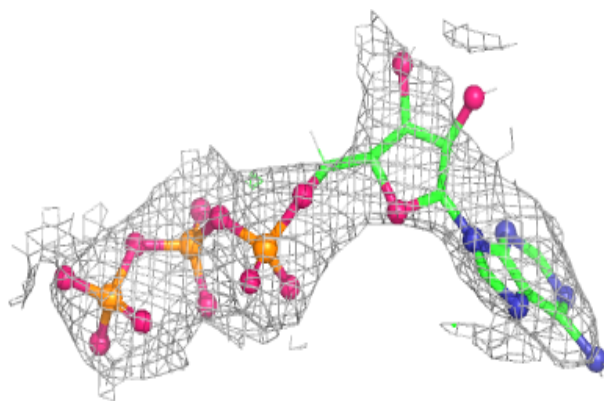
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	E	301	5/5	0.80	0.32	102,106,113,114	0
3	SO4	F	301	5/5	0.83	0.28	88,92,93,99	0
3	SO4	B	301	5/5	0.84	0.26	92,93,98,99	0
3	SO4	D	301	5/5	0.87	0.30	144,145,149,151	0
4	ATP	P	301	31/31	0.90	0.27	67,129,164,168	0
3	SO4	G	301	5/5	0.91	0.20	112,117,118,119	0
3	SO4	N	302	5/5	0.93	0.20	38,38,38,38	0
3	SO4	M	301	5/5	0.94	0.26	67,72,75,90	0
4	ATP	A	301	31/31	0.96	0.18	33,41,53,54	0
3	SO4	Q	301	5/5	0.96	0.29	97,103,105,106	0
3	SO4	N	301	5/5	0.97	0.20	64,73,79,80	0
3	SO4	R	301	5/5	0.97	0.18	44,44,44,44	0
5	CL	M	302	1/1	0.97	0.22	38,38,38,38	0

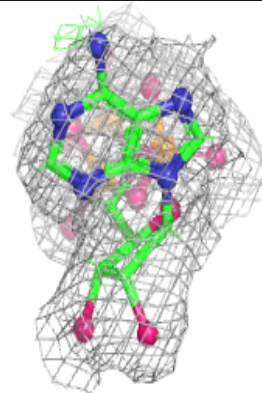
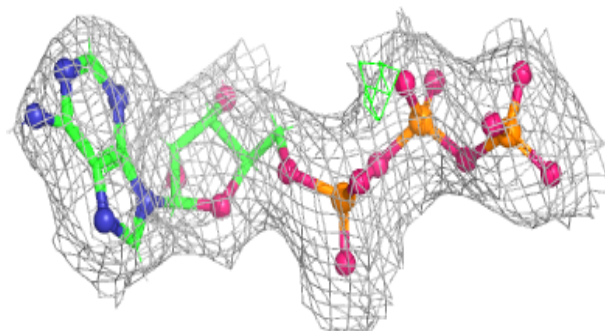
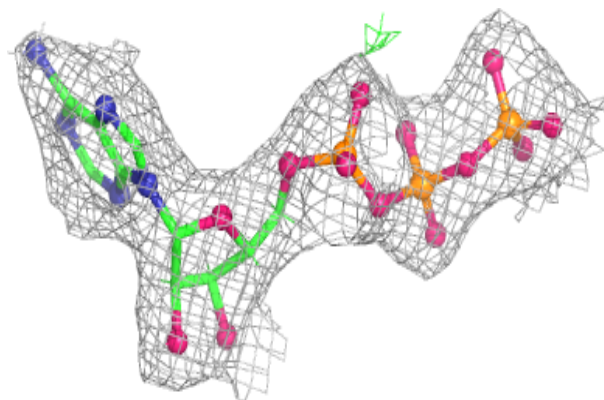
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP P 301:

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

**Electron density around ATP A 301:**

$2mF_o-DF_c$ (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.