



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:15 PM UTC

PDB ID : 4YTX / pdb_00004ytx
Title : Crystal structure of Ups1-Mdm35 complex with PA
Authors : Watanabe, Y.; Tamura, Y.; Kawano, S.; Endo, T.
Deposited on : 2015-03-18
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

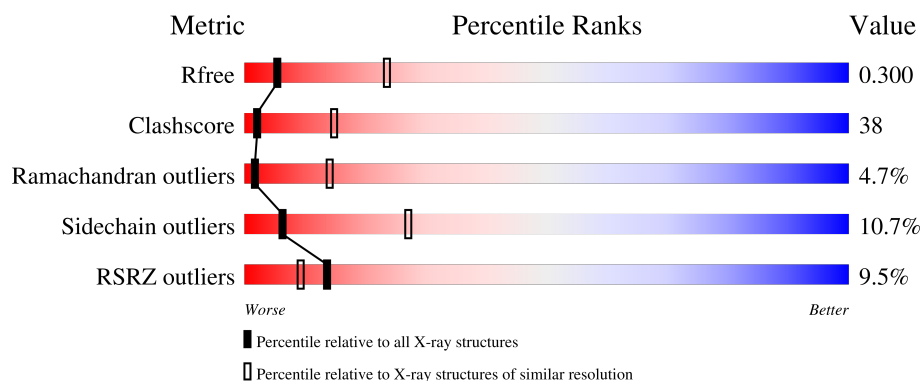
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	81	
1	C	81	
1	E	81	
1	G	81	
1	I	81	

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Mol	Chain	Length	Quality of chain
1	K	81	
1	M	81	
1	O	81	
2	B	184	
2	D	184	
2	F	184	
2	H	184	
2	J	184	
2	L	184	
2	N	184	
2	P	184	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15084 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mitochondrial distribution and morphology protein 35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	73	Total	C	N	O	S	0	0	0
			584	372	91	116	5			
1	C	73	Total	C	N	O	S	0	0	0
			580	370	91	114	5			
1	E	73	Total	C	N	O	S	0	0	0
			584	372	91	116	5			
1	G	73	Total	C	N	O	S	0	0	0
			584	372	91	116	5			
1	I	73	Total	C	N	O	S	0	0	0
			584	372	91	116	5			
1	K	73	Total	C	N	O	S	0	0	0
			584	372	91	116	5			
1	M	73	Total	C	N	O	S	0	0	0
			584	372	91	116	5			
1	O	68	Total	C	N	O	S	0	0	0
			551	352	86	109	4			

- Molecule 2 is a protein called Protein UPS1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1278	811	222	241	4			
2	D	170	Total	C	N	O	S	0	0	0
			1344	849	233	256	6			
2	F	167	Total	C	N	O	S	0	0	0
			1325	838	230	253	4			
2	H	162	Total	C	N	O	S	0	0	0
			1249	794	214	236	5			
2	J	169	Total	C	N	O	S	0	0	0
			1332	844	229	254	5			
2	L	169	Total	C	N	O	S	0	0	0
			1330	842	229	254	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	157	Total	C	N	O	S	0	0	0
			1257	792	218	242	5			
2	P	159	Total	C	N	O	S	0	0	0
			1262	796	218	243	5			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	expression tag	UNP Q05776
B	-12	GLY	-	expression tag	UNP Q05776
B	-11	SER	-	expression tag	UNP Q05776
B	-10	SER	-	expression tag	UNP Q05776
B	-9	HIS	-	expression tag	UNP Q05776
B	-8	HIS	-	expression tag	UNP Q05776
B	-7	HIS	-	expression tag	UNP Q05776
B	-6	HIS	-	expression tag	UNP Q05776
B	-5	HIS	-	expression tag	UNP Q05776
B	-4	HIS	-	expression tag	UNP Q05776
B	-3	SER	-	expression tag	UNP Q05776
B	-2	GLN	-	expression tag	UNP Q05776
B	-1	ASP	-	expression tag	UNP Q05776
B	0	PRO	-	expression tag	UNP Q05776
D	-13	MET	-	expression tag	UNP Q05776
D	-12	GLY	-	expression tag	UNP Q05776
D	-11	SER	-	expression tag	UNP Q05776
D	-10	SER	-	expression tag	UNP Q05776
D	-9	HIS	-	expression tag	UNP Q05776
D	-8	HIS	-	expression tag	UNP Q05776
D	-7	HIS	-	expression tag	UNP Q05776
D	-6	HIS	-	expression tag	UNP Q05776
D	-5	HIS	-	expression tag	UNP Q05776
D	-4	HIS	-	expression tag	UNP Q05776
D	-3	SER	-	expression tag	UNP Q05776
D	-2	GLN	-	expression tag	UNP Q05776
D	-1	ASP	-	expression tag	UNP Q05776
D	0	PRO	-	expression tag	UNP Q05776
F	-13	MET	-	expression tag	UNP Q05776
F	-12	GLY	-	expression tag	UNP Q05776
F	-11	SER	-	expression tag	UNP Q05776
F	-10	SER	-	expression tag	UNP Q05776
F	-9	HIS	-	expression tag	UNP Q05776
F	-8	HIS	-	expression tag	UNP Q05776

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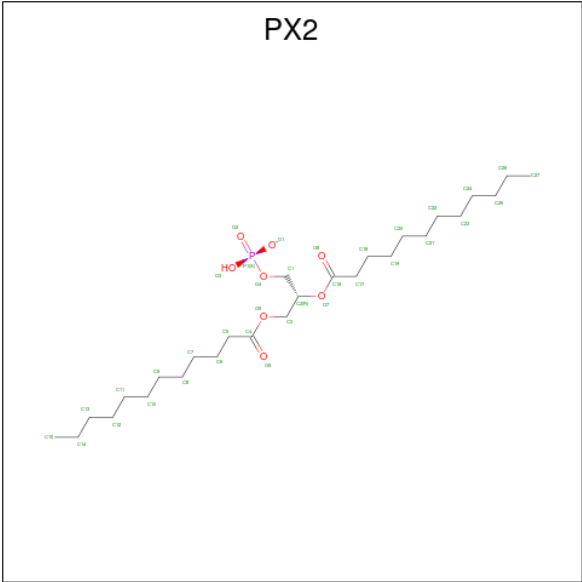
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F	-5	HIS	-	expression tag	UNP Q05776
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F	-3	SER	-	expression tag	UNP Q05776
F	-2	GLN	-	expression tag	UNP Q05776
F	-1	ASP	-	expression tag	UNP Q05776
F	0	PRO	-	expression tag	UNP Q05776
H	-13	MET	-	expression tag	UNP Q05776
H	-12	GLY	-	expression tag	UNP Q05776
H	-11	SER	-	expression tag	UNP Q05776
H	-10	SER	-	expression tag	UNP Q05776
H	-9	HIS	-	expression tag	UNP Q05776
H	-8	HIS	-	expression tag	UNP Q05776
H	-7	HIS	-	expression tag	UNP Q05776
H	-6	HIS	-	expression tag	UNP Q05776
H	-5	HIS	-	expression tag	UNP Q05776
H	-4	HIS	-	expression tag	UNP Q05776
H	-3	SER	-	expression tag	UNP Q05776
H	-2	GLN	-	expression tag	UNP Q05776
H	-1	ASP	-	expression tag	UNP Q05776
H	0	PRO	-	expression tag	UNP Q05776
J	-13	MET	-	expression tag	UNP Q05776
J	-12	GLY	-	expression tag	UNP Q05776
J	-11	SER	-	expression tag	UNP Q05776
J	-10	SER	-	expression tag	UNP Q05776
J	-9	HIS	-	expression tag	UNP Q05776
J	-8	HIS	-	expression tag	UNP Q05776
J	-7	HIS	-	expression tag	UNP Q05776
J	-6	HIS	-	expression tag	UNP Q05776
J	-5	HIS	-	expression tag	UNP Q05776
J	-4	HIS	-	expression tag	UNP Q05776
J	-3	SER	-	expression tag	UNP Q05776
J	-2	GLN	-	expression tag	UNP Q05776
J	-1	ASP	-	expression tag	UNP Q05776
J	0	PRO	-	expression tag	UNP Q05776
L	-13	MET	-	expression tag	UNP Q05776
L	-12	GLY	-	expression tag	UNP Q05776
L	-11	SER	-	expression tag	UNP Q05776
L	-10	SER	-	expression tag	UNP Q05776
L	-9	HIS	-	expression tag	UNP Q05776
L	-8	HIS	-	expression tag	UNP Q05776

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-7	HIS	-	expression tag	UNP Q05776
L	-6	HIS	-	expression tag	UNP Q05776
L	-5	HIS	-	expression tag	UNP Q05776
L	-4	HIS	-	expression tag	UNP Q05776
L	-3	SER	-	expression tag	UNP Q05776
L	-2	GLN	-	expression tag	UNP Q05776
L	-1	ASP	-	expression tag	UNP Q05776
L	0	PRO	-	expression tag	UNP Q05776
N	-13	MET	-	expression tag	UNP Q05776
N	-12	GLY	-	expression tag	UNP Q05776
N	-11	SER	-	expression tag	UNP Q05776
N	-10	SER	-	expression tag	UNP Q05776
N	-9	HIS	-	expression tag	UNP Q05776
N	-8	HIS	-	expression tag	UNP Q05776
N	-7	HIS	-	expression tag	UNP Q05776
N	-6	HIS	-	expression tag	UNP Q05776
N	-5	HIS	-	expression tag	UNP Q05776
N	-4	HIS	-	expression tag	UNP Q05776
N	-3	SER	-	expression tag	UNP Q05776
N	-2	GLN	-	expression tag	UNP Q05776
N	-1	ASP	-	expression tag	UNP Q05776
N	0	PRO	-	expression tag	UNP Q05776
P	-13	MET	-	expression tag	UNP Q05776
P	-12	GLY	-	expression tag	UNP Q05776
P	-11	SER	-	expression tag	UNP Q05776
P	-10	SER	-	expression tag	UNP Q05776
P	-9	HIS	-	expression tag	UNP Q05776
P	-8	HIS	-	expression tag	UNP Q05776
P	-7	HIS	-	expression tag	UNP Q05776
P	-6	HIS	-	expression tag	UNP Q05776
P	-5	HIS	-	expression tag	UNP Q05776
P	-4	HIS	-	expression tag	UNP Q05776
P	-3	SER	-	expression tag	UNP Q05776
P	-2	GLN	-	expression tag	UNP Q05776
P	-1	ASP	-	expression tag	UNP Q05776
P	0	PRO	-	expression tag	UNP Q05776

- Molecule 3 is 1,2-DILAULOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).

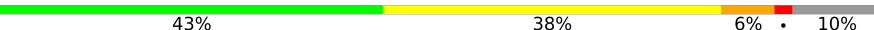


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			36	27	8	1		
3	F	1	Total	C	O	P	0	0
			36	27	8	1		

3 Residue-property plots [i](#)

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.

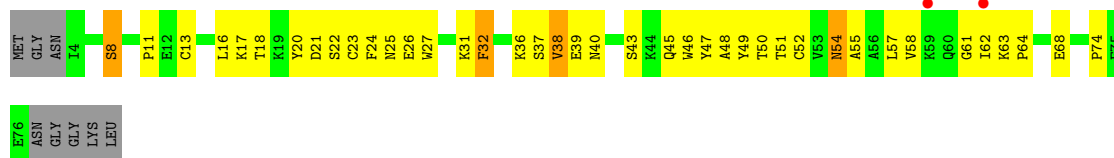
- Molecule 1: Mitochondrial distribution and morphology protein 35

Chain A: 



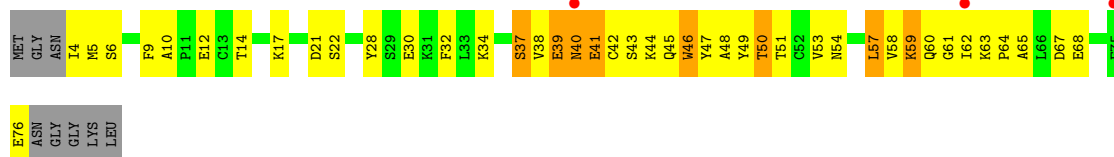
- Molecule 1: Mitochondrial distribution and morphology protein 35

Chain C: 

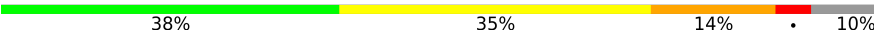


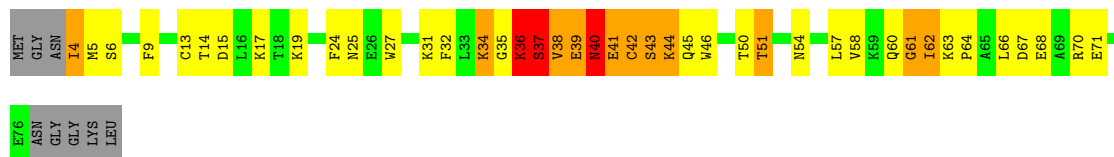
- Molecule 1: Mitochondrial distribution and morphology protein 35

Chain E: 

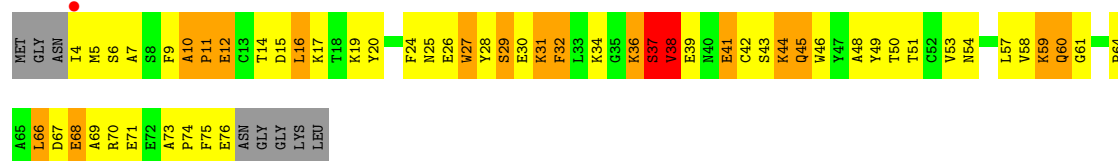
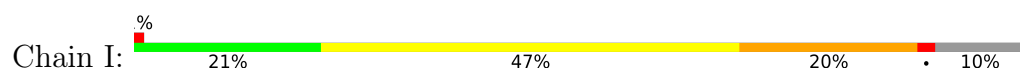


- Molecule 1: Mitochondrial distribution and morphology protein 35

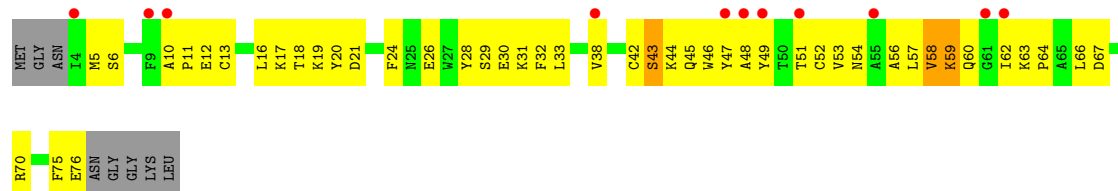
Chain G: 



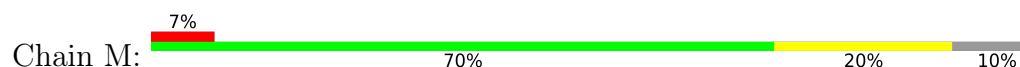
- Molecule 1: Mitochondrial distribution and morphology protein 35



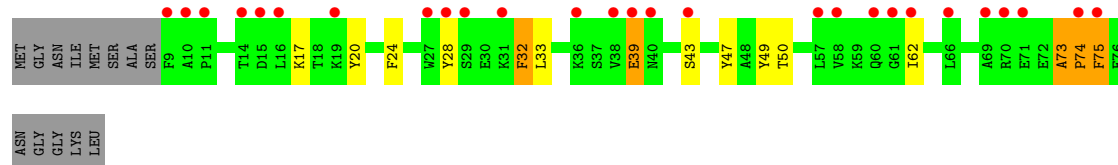
- Molecule 1: Mitochondrial distribution and morphology protein 35



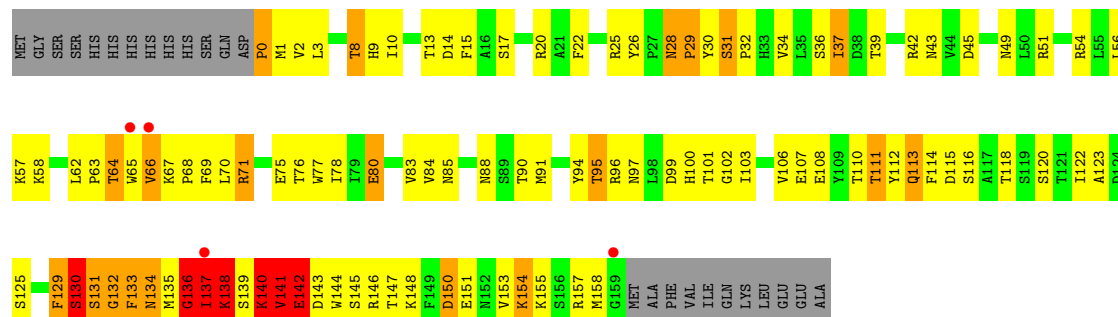
- Molecule 1: Mitochondrial distribution and morphology protein 35



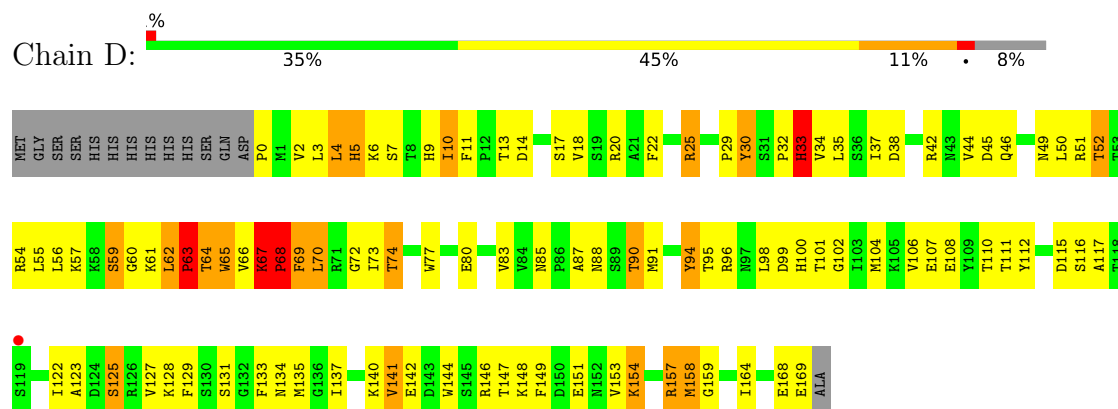
- Molecule 1: Mitochondrial distribution and morphology protein 35



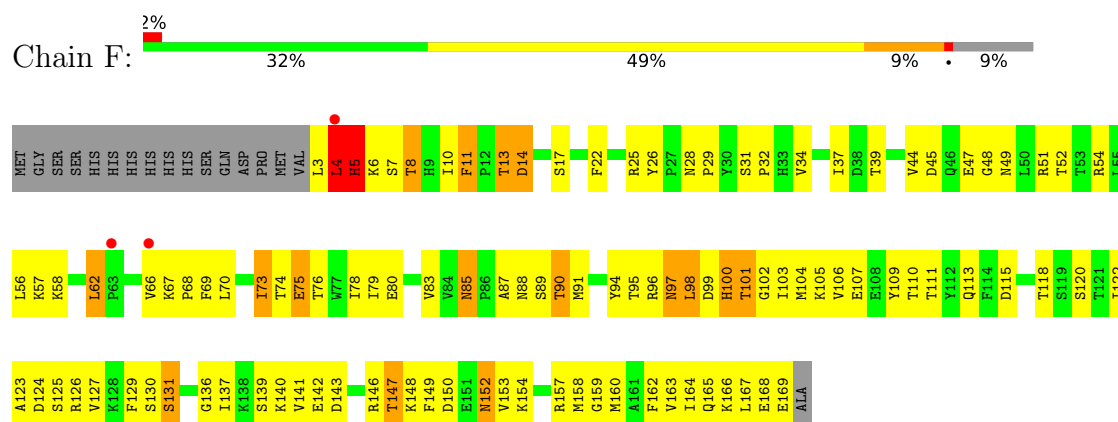
- Molecule 2: Protein UPS1, mitochondrial



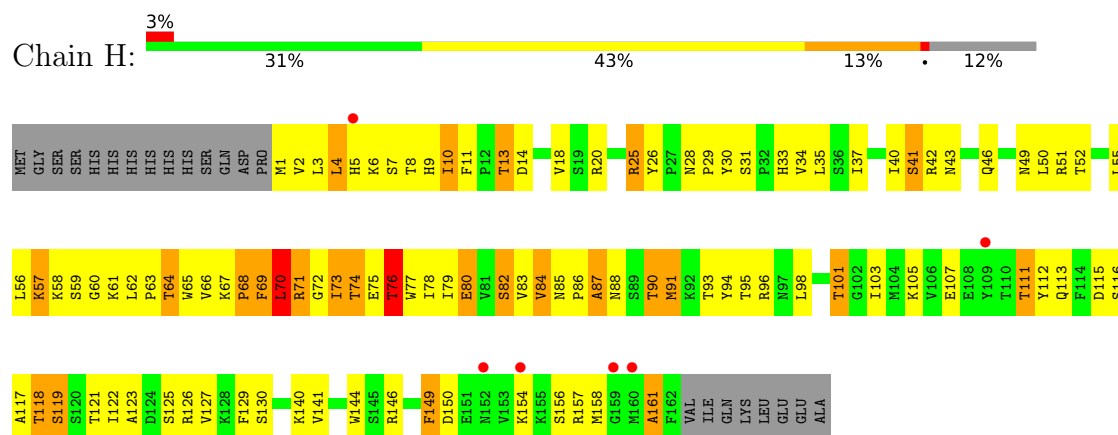
• Molecule 2: Protein UPS1, mitochondrial



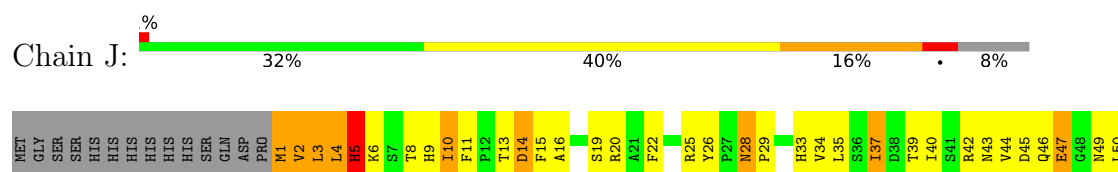
• Molecule 2: Protein UPS1, mitochondrial

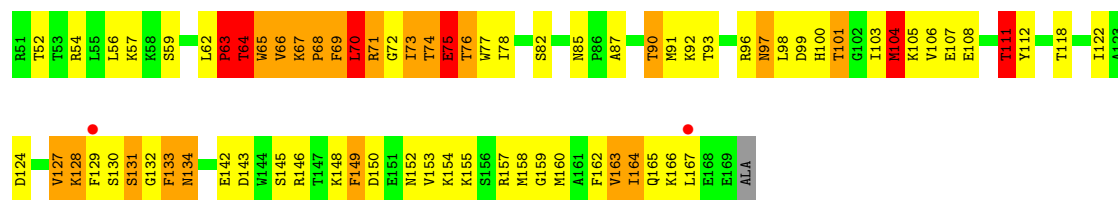


• Molecule 2: Protein UPS1, mitochondrial

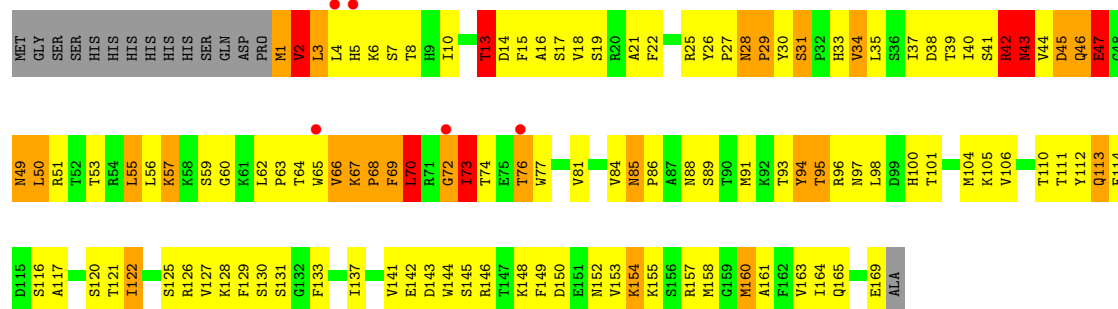


• Molecule 2: Protein UPS1, mitochondrial

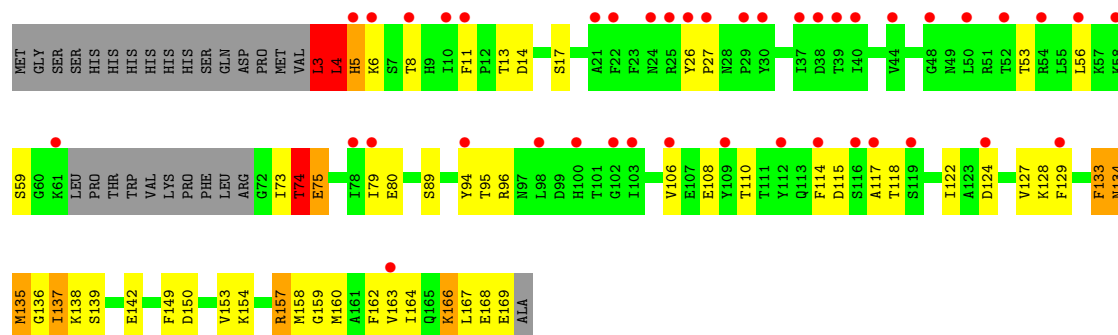




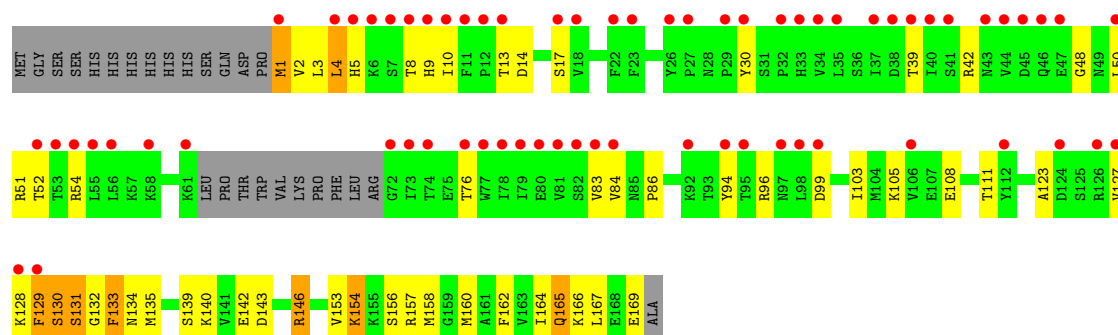
• Molecule 2: Protein UPS1, mitochondrial



• Molecule 2: Protein UPS1, mitochondrial



• Molecule 2: Protein UPS1, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.64Å 154.67Å 99.01Å 90.00° 104.42° 90.00°	Depositor
Resolution (Å)	43.23 – 3.20 43.23 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (43.23-3.20) 94.6 (43.23-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 3.19Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.251 , 0.300 0.251 , 0.300	Depositor DCC
R_{free} test set	4772 reflections (9.44%)	wwPDB-VP
Wilson B-factor (Å ²)	68.9	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15084	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: PX2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/598	1.08	3/807 (0.4%)
1	C	0.65	0/594	1.05	4/802 (0.5%)
1	E	0.53	0/598	0.95	3/807 (0.4%)
1	G	1.80	20/598 (3.3%)	1.53	15/807 (1.9%)
1	I	0.50	0/598	1.32	10/807 (1.2%)
1	K	0.39	0/598	0.89	1/807 (0.1%)
1	M	0.43	0/598	0.91	1/807 (0.1%)
1	O	0.39	0/565	1.10	4/763 (0.5%)
2	B	1.48	27/1308 (2.1%)	1.35	20/1771 (1.1%)
2	D	0.73	0/1373	1.32	16/1858 (0.9%)
2	F	0.63	0/1355	1.06	10/1835 (0.5%)
2	H	0.59	0/1280	1.20	15/1742 (0.9%)
2	J	1.76	41/1362 (3.0%)	1.49	23/1847 (1.2%)
2	L	0.58	0/1359	1.28	20/1841 (1.1%)
2	N	0.54	0/1282	0.98	6/1729 (0.3%)
2	P	0.47	0/1287	0.91	2/1738 (0.1%)
All	All	0.92	88/15353 (0.6%)	1.19	153/20768 (0.7%)

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	G	0	3
2	B	0	5
2	F	0	1
2	J	0	4
All	All	0	13

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	76	THR	C-O	-23.38	0.93	1.23
2	J	77	TRP	C-O	-18.17	1.02	1.23
2	B	130	SER	C-O	-17.70	1.08	1.24
2	J	77	TRP	CA-C	-14.84	1.34	1.52
2	B	130	SER	CA-CB	-14.20	1.35	1.54
1	G	43	SER	CA-C	-12.98	1.39	1.53
1	G	37	SER	CA-C	-12.90	1.35	1.53
2	B	130	SER	CA-C	-11.96	1.39	1.53
2	J	77	TRP	CD2-CE2	-11.68	1.21	1.41
1	G	34	LYS	C-O	-11.09	1.09	1.24
2	B	131	SER	C-O	-10.94	1.10	1.23
2	B	133	PHE	C-O	-10.78	1.10	1.24
2	J	75	GLU	CA-C	-10.61	1.37	1.53
2	J	71	ARG	C-O	-10.59	1.10	1.24
1	G	40	ASN	CA-C	-10.56	1.38	1.52
1	G	41	GLU	N-CA	-9.73	1.34	1.46
2	J	74	THR	C-O	-9.45	1.12	1.24
2	J	77	TRP	CZ3-CH2	-9.45	1.16	1.40
2	J	75	GLU	C-O	-9.24	1.10	1.24
1	G	36	LYS	CA-C	-9.22	1.40	1.53
1	G	37	SER	C-O	-9.19	1.11	1.23
2	J	75	GLU	CA-CB	-9.12	1.38	1.53
2	J	76	THR	CA-C	-9.11	1.40	1.52
2	J	74	THR	CA-CB	-9.10	1.38	1.53
2	J	66	VAL	N-CA	-9.02	1.35	1.46
2	B	138	LYS	C-O	-8.88	1.13	1.24
2	J	67	LYS	CA-C	-8.85	1.41	1.52
2	B	137	ILE	N-CA	-8.83	1.36	1.46
2	B	133	PHE	N-CA	-8.81	1.34	1.46
2	B	142	GLU	CA-C	-8.81	1.41	1.52
1	G	43	SER	CA-CB	-8.76	1.42	1.53
1	G	42	CYS	C-O	-8.36	1.16	1.24
1	G	40	ASN	C-O	-8.31	1.14	1.23
2	J	69	PHE	C-O	-8.29	1.13	1.24
2	B	134	ASN	CA-C	-8.14	1.41	1.52
2	B	139	SER	CA-C	-8.07	1.42	1.52
2	J	66	VAL	CA-CB	-7.97	1.43	1.54
1	G	43	SER	C-O	-7.97	1.15	1.23
2	J	76	THR	C-N	-7.89	1.22	1.33
1	G	34	LYS	CA-C	-7.81	1.42	1.52
2	J	76	THR	CB-CG2	-7.64	1.27	1.52
2	J	73	ILE	N-CA	-7.57	1.36	1.46
2	B	132	GLY	C-O	-7.50	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	76	THR	CA-CB	-7.20	1.42	1.53
2	B	138	LYS	CA-C	-7.17	1.43	1.52
2	J	77	TRP	CE3-CZ3	-7.07	1.17	1.38
2	J	77	TRP	CD1-NE1	-7.05	1.23	1.37
2	J	71	ARG	CA-C	-7.05	1.42	1.52
2	J	68	PRO	CA-C	-7.00	1.42	1.52
2	J	74	THR	CB-CG2	-6.99	1.29	1.52
2	B	130	SER	CB-OG	-6.90	1.28	1.42
2	J	77	TRP	CE2-CZ2	-6.75	1.25	1.39
1	G	36	LYS	N-CA	-6.64	1.37	1.45
1	G	34	LYS	C-N	-6.63	1.25	1.34
2	B	141	VAL	N-CA	-6.55	1.38	1.46
2	J	75	GLU	N-CA	-6.36	1.36	1.45
2	J	68	PRO	C-O	-6.32	1.16	1.24
2	J	68	PRO	CA-CB	-6.29	1.44	1.53
1	G	41	GLU	CA-CB	-6.25	1.42	1.53
2	B	131	SER	CA-C	-6.15	1.45	1.52
2	B	139	SER	N-CA	-6.04	1.39	1.46
2	J	77	TRP	N-CA	-6.03	1.38	1.46
2	J	66	VAL	CA-C	-5.96	1.45	1.52
2	J	67	LYS	C-O	-5.94	1.16	1.24
2	J	77	TRP	CG-CD1	-5.91	1.22	1.36
2	J	77	TRP	CG-CD2	-5.83	1.33	1.43
2	J	70	LEU	CA-C	-5.81	1.43	1.52
2	J	73	ILE	C-O	-5.77	1.17	1.24
2	J	77	TRP	C-N	-5.71	1.25	1.33
2	J	74	THR	CA-C	-5.66	1.45	1.52
2	B	142	GLU	C-N	-5.63	1.26	1.34
2	B	137	ILE	C-O	-5.59	1.17	1.24
2	J	66	VAL	C-O	-5.56	1.17	1.24
1	G	39	GLU	CA-C	5.46	1.59	1.52
1	G	42	CYS	N-CA	-5.45	1.39	1.46
2	J	74	THR	CB-OG1	-5.42	1.35	1.43
2	B	139	SER	CA-CB	-5.42	1.44	1.53
2	B	131	SER	CA-CB	-5.33	1.44	1.53
1	G	36	LYS	C-O	-5.31	1.16	1.23
2	B	136	GLY	C-O	-5.31	1.16	1.23
2	B	137	ILE	CA-C	-5.30	1.46	1.52
2	B	141	VAL	CA-C	-5.30	1.46	1.52
1	G	38	VAL	N-CA	-5.28	1.39	1.46
2	B	131	SER	N-CA	-5.10	1.39	1.45
2	B	140	LYS	C-N	-5.10	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	39	GLU	N-CA	5.09	1.52	1.45
2	J	65	TRP	C-N	-5.06	1.26	1.33
2	B	135	MET	N-CA	-5.03	1.40	1.46

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	73	ILE	N-CA-C	-18.36	80.94	107.75
1	I	37	SER	N-CA-C	17.91	132.44	110.41
2	L	73	ILE	N-CA-C	14.34	125.68	110.05
2	D	4	LEU	N-CA-C	14.09	127.67	108.23
2	J	4	LEU	N-CA-C	13.84	127.33	108.23
2	J	65	TRP	N-CA-C	-13.44	96.85	113.38
2	L	72	GLY	N-CA-C	-12.34	87.03	111.34
2	B	130	SER	CA-CB-OG	-12.13	86.83	111.10
2	D	74	THR	N-CA-C	-11.86	98.53	113.23
1	O	73	ALA	CA-C-N	11.85	131.75	119.19
1	O	73	ALA	C-N-CA	11.85	131.75	119.19
2	D	67	LYS	N-CA-C	-11.42	84.58	109.81
1	G	36	LYS	N-CA-C	-11.20	96.08	110.53
2	N	4	LEU	N-CA-C	10.18	132.48	110.80
2	J	75	GLU	N-CA-C	-10.06	94.07	109.96
2	B	142	GLU	CA-C-N	-9.97	105.83	120.38
2	B	142	GLU	C-N-CA	-9.97	105.83	120.38
2	H	6	LYS	N-CA-C	9.84	123.84	110.55
2	J	73	ILE	CA-C-N	9.63	133.97	120.29
2	J	73	ILE	C-N-CA	9.63	133.97	120.29
2	B	133	PHE	CA-C-N	9.42	139.53	121.54
2	B	133	PHE	C-N-CA	9.42	139.53	121.54
2	B	130	SER	CA-C-O	-8.30	112.09	120.80
2	L	65	TRP	N-CA-C	-8.24	102.48	112.54
2	L	34	VAL	N-CA-C	-8.20	101.11	110.05
2	J	76	THR	O-C-N	-8.12	114.95	123.56
2	B	142	GLU	CA-C-O	8.05	129.28	120.82
2	D	67	LYS	CA-C-N	8.04	129.89	119.84
2	D	67	LYS	C-N-CA	8.04	129.89	119.84
1	G	62	ILE	N-CA-C	8.01	118.56	110.23
2	J	74	THR	CA-CB-OG1	-7.91	97.74	109.60
1	G	35	GLY	CA-C-O	7.87	126.40	119.56
1	O	74	PRO	N-CA-C	7.84	123.84	113.57
2	H	70	LEU	N-CA-C	-7.65	94.50	110.80
2	D	72	GLY	N-CA-C	-7.52	95.35	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	142	GLU	CB-CA-C	-7.45	99.18	110.88
2	H	154	LYS	N-CA-C	-7.01	104.53	113.23
2	L	81	VAL	N-CA-C	6.98	116.77	106.85
2	L	47	GLU	N-CA-C	6.93	121.41	112.26
2	D	61	LYS	N-CA-C	6.92	119.76	110.35
1	I	68	GLU	N-CA-C	-6.89	103.21	111.69
2	H	74	THR	N-CA-C	-6.81	104.07	112.38
1	G	42	CYS	N-CA-CB	-6.81	103.62	111.79
1	I	38	VAL	N-CA-C	6.71	123.30	109.34
2	F	5	HIS	N-CA-C	-6.69	96.56	110.80
1	G	40	ASN	N-CA-CB	6.68	119.90	109.69
2	P	130	SER	N-CA-C	6.66	118.27	108.14
2	B	142	GLU	N-CA-C	-6.64	103.96	111.07
1	C	32	PHE	N-CA-C	6.64	118.17	111.07
2	B	150	ASP	N-CA-C	-6.63	104.29	112.38
2	D	4	LEU	CA-C-N	6.62	134.19	121.54
2	D	4	LEU	C-N-CA	6.62	134.19	121.54
1	G	39	GLU	N-CA-C	6.61	119.76	109.52
2	J	76	THR	OG1-CB-CG2	-6.58	96.13	109.30
2	H	156	SER	N-CA-C	-6.58	103.74	113.61
1	G	36	LYS	CA-C-O	-6.58	114.37	121.94
2	F	125	SER	N-CA-C	6.58	119.13	108.34
2	J	67	LYS	CB-CA-C	-6.57	97.23	110.17
2	L	42	ARG	N-CA-C	-6.55	101.88	110.53
1	C	52	CYS	N-CA-C	-6.54	103.78	111.03
2	F	97	ASN	N-CA-C	-6.51	101.49	110.35
2	N	159	GLY	N-CA-C	-6.50	104.62	112.49
2	D	158	MET	N-CA-C	-6.49	104.29	111.82
1	I	60	GLN	N-CA-C	-6.46	101.39	110.50
2	J	68	PRO	CB-CA-C	-6.44	102.00	112.62
1	G	42	CYS	CB-CA-C	6.42	121.77	111.24
2	F	4	LEU	N-CA-C	6.38	124.39	110.80
2	B	0	PRO	N-CA-CB	6.34	109.98	103.00
1	M	32	PHE	N-CA-C	6.33	118.71	111.11
2	N	3	LEU	CA-C-N	6.26	133.50	121.54
2	N	3	LEU	C-N-CA	6.26	133.50	121.54
2	L	85	ASN	CA-C-N	6.25	127.65	119.84
2	L	85	ASN	C-N-CA	6.25	127.65	119.84
2	B	142	GLU	N-CA-CB	-6.25	100.95	110.01
2	J	10	ILE	N-CA-C	6.23	116.90	108.17
1	I	45	GLN	N-CA-C	-6.23	106.00	113.97
2	J	4	LEU	CA-C-N	6.21	133.41	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	4	LEU	C-N-CA	6.21	133.41	121.54
1	C	54	ASN	N-CA-C	6.16	117.66	111.07
2	D	0	PRO	N-CA-CB	6.13	109.75	103.00
2	B	140	LYS	N-CA-C	-6.11	104.53	111.07
2	J	5	HIS	N-CA-C	-6.05	97.92	110.80
2	F	11	PHE	N-CA-C	-6.04	102.46	110.07
2	B	140	LYS	CD-CE-NZ	6.01	131.15	111.90
1	G	42	CYS	N-CA-C	6.01	117.51	110.41
2	F	4	LEU	CA-C-N	6.00	133.00	121.54
2	F	4	LEU	C-N-CA	6.00	133.00	121.54
1	G	36	LYS	CA-C-N	5.94	131.78	120.97
1	G	36	LYS	C-N-CA	5.94	131.78	120.97
2	B	140	LYS	CA-C-N	5.89	128.53	120.46
2	B	140	LYS	C-N-CA	5.89	128.53	120.46
1	E	28	TYR	N-CA-C	5.87	117.48	111.14
2	L	122	ILE	N-CA-C	5.84	116.21	107.51
2	L	76	THR	N-CA-C	5.81	118.76	110.10
1	K	31	LYS	N-CA-C	5.80	119.17	111.75
2	L	60	GLY	N-CA-C	-5.75	103.81	112.89
1	A	39	GLU	N-CA-C	5.73	123.01	110.80
2	L	66	VAL	N-CA-C	-5.72	99.58	108.44
2	P	146	ARG	N-CA-C	-5.71	104.69	111.03
2	L	127	VAL	N-CA-C	5.67	115.77	107.37
2	H	125	SER	N-CA-C	5.66	118.01	107.99
1	I	37	SER	CA-C-N	5.62	132.08	121.97
1	I	37	SER	C-N-CA	5.62	132.08	121.97
1	A	8	SER	N-CA-C	-5.61	102.22	110.52
1	A	60	GLN	N-CA-C	5.61	117.83	109.25
2	J	68	PRO	CA-N-CD	-5.61	104.15	112.00
1	E	59	LYS	N-CA-C	-5.60	107.03	112.97
2	H	150	ASP	N-CA-C	-5.60	106.29	113.01
2	B	129	PHE	O-C-N	-5.58	116.69	123.10
2	H	157	ARG	N-CA-C	-5.57	106.52	113.38
1	E	32	PHE	N-CA-C	5.54	117.76	111.11
2	H	119	SER	N-CA-C	-5.52	106.49	113.23
2	D	154	LYS	N-CA-C	-5.51	104.49	111.11
2	F	14	ASP	N-CA-C	5.51	117.95	110.35
2	J	64	THR	N-CA-C	5.46	124.55	113.20
2	N	136	GLY	N-CA-C	-5.41	106.24	112.73
2	J	74	THR	N-CA-CB	-5.40	102.17	110.16
2	L	62	LEU	CA-C-N	5.39	126.58	119.84
2	L	62	LEU	C-N-CA	5.39	126.58	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	77	TRP	CA-CB-CG	5.39	123.83	113.60
1	G	41	GLU	N-CA-CB	-5.38	103.27	111.66
2	J	71	ARG	N-CA-C	-5.38	106.42	112.87
1	O	32	PHE	N-CA-C	5.36	116.80	111.07
1	G	37	SER	N-CA-C	-5.33	103.49	110.53
1	G	71	GLU	N-CA-C	-5.33	106.62	113.01
2	N	6	LYS	N-CA-C	5.32	117.36	107.99
1	C	8	SER	N-CA-C	-5.32	103.36	110.55
1	I	10	ALA	CA-C-N	5.32	126.49	119.84
1	I	10	ALA	C-N-CA	5.32	126.49	119.84
2	J	75	GLU	CA-C-O	-5.31	114.39	121.46
2	J	111	THR	N-CA-C	5.29	116.95	107.80
1	I	59	LYS	N-CA-C	-5.28	105.22	110.97
2	D	64	THR	N-CA-C	5.28	122.04	110.80
2	J	73	ILE	CA-C-O	-5.25	114.93	120.39
2	B	28	ASN	CA-C-N	5.22	126.36	119.84
2	B	28	ASN	C-N-CA	5.22	126.36	119.84
2	D	159	GLY	N-CA-C	-5.20	106.11	112.77
2	L	160	MET	N-CA-C	-5.20	105.53	111.14
1	G	9	PHE	N-CA-C	-5.19	105.80	111.82
2	H	10	ILE	N-CA-C	5.18	115.31	107.75
2	L	53	THR	N-CA-C	-5.12	100.35	109.06
2	H	76	THR	N-CA-C	5.11	117.93	109.85
2	D	68	PRO	CA-N-CD	-5.09	104.87	112.00
2	H	4	LEU	N-CA-C	5.09	118.25	110.36
2	B	137	ILE	CB-CA-C	-5.07	105.48	111.97
2	H	73	ILE	N-CA-C	5.07	119.88	109.34
2	L	106	VAL	N-CA-C	5.06	114.89	107.15
2	L	122	ILE	CB-CA-C	-5.05	104.24	111.31
2	D	30	TYR	N-CA-C	5.05	117.90	111.69
2	F	85	ASN	CA-C-N	5.03	125.10	119.87
2	F	85	ASN	C-N-CA	5.03	125.10	119.87
2	H	103	ILE	N-CA-C	-5.03	107.95	113.43
2	H	161	ALA	N-CA-C	-5.02	107.11	113.18

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	133	PHE	Peptide
2	B	136	GLY	Peptide
2	B	138	LYS	Mainchain

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Mol	Chain	Res	Type	Group
2	B	140	LYS	Mainchain
2	B	142	GLU	Mainchain
2	F	109	TYR	Sidechain
1	G	36	LYS	Peptide
1	G	37	SER	Peptide
1	G	40	ASN	Mainchain
2	J	70	LEU	Peptide
2	J	73	ILE	Peptide,Mainchain
2	J	75	GLU	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	584	0	551	29	0
1	C	580	0	547	24	0
1	E	584	0	551	41	0
1	G	584	0	551	41	0
1	I	584	0	551	64	0
1	K	584	0	551	59	0
1	M	584	0	551	9	0
1	O	551	0	516	14	0
2	B	1278	0	1265	137	0
2	D	1344	0	1313	122	0
2	F	1325	0	1296	135	0
2	H	1249	0	1178	111	0
2	J	1332	0	1300	156	0
2	L	1330	0	1298	145	0
2	N	1257	0	1241	77	0
2	P	1262	0	1240	75	0
3	B	36	0	52	8	0
3	F	36	0	52	7	0
All	All	15084	0	14604	1117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (1117) 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)
2:H:158:MET:SD	2:N:122:ILE:HD11	1.82	1.19
2:B:102:GLY:O	2:B:132:GLY:HA3	1.44	1.18
2:J:163:VAL:HG21	2:L:25:ARG:HA	1.37	1.06
2:D:9:HIS:HD2	2:J:8:THR:HG23	1.20	1.06
1:G:40:ASN:OD1	1:G:42:CYS:N	1.91	1.03
2:P:2:VAL:HG22	2:P:130:SER:HB3	1.40	1.01
1:E:60:GLN:HB3	1:E:62:ILE:HG22	1.42	0.99
2:J:1:MET:O	2:J:2:VAL:HG13	1.64	0.97
2:F:39:THR:HA	2:F:54:ARG:HG2	1.45	0.97
2:F:80:GLU:HA	2:F:95:THR:HG22	1.47	0.97
2:B:140:LYS:O	2:B:143:ASP:CG	2.09	0.95
2:H:84:VAL:HG22	2:H:91:MET:CE	1.95	0.95
1:I:38:VAL:HG13	1:I:39:GLU:H	1.29	0.94
1:G:43:SER:O	1:G:45:GLN:N	2.01	0.94
2:L:73:ILE:H	2:L:73:ILE:HD12	1.32	0.94
2:D:3:LEU:C	2:D:4:LEU:HD22	1.93	0.94
2:B:97:ASN:HB3	3:B:201:PX2:H15	1.51	0.93
2:B:8:THR:HG22	2:H:7:SER:HB2	1.52	0.92
2:H:35:LEU:HD11	2:H:59:SER:HB3	1.52	0.92
2:J:149:PHE:HZ	2:L:7:SER:HB2	1.33	0.92
2:B:9:HIS:HD2	2:H:8:THR:HG23	1.33	0.91
2:D:3:LEU:O	2:D:4:LEU:HD22	1.71	0.90
2:N:5:HIS:HD1	2:N:129:PHE:HE1	1.09	0.90
2:P:4:LEU:HB2	2:P:127:VAL:O	1.70	0.90
2:B:137:ILE:O	2:B:140:LYS:N	2.04	0.90
2:L:45:ASP:OD1	2:L:51:ARG:HD3	1.72	0.89
2:J:66:VAL:O	2:J:68:PRO:HG2	1.72	0.89
1:I:31:LYS:HD2	1:I:36:LYS:HG2	1.55	0.89
2:D:67:LYS:N	2:D:68:PRO:CD	2.34	0.88
2:L:1:MET:O	2:L:2:VAL:HG23	1.73	0.88
2:N:149:PHE:O	2:N:153:VAL:HG23	1.72	0.88
2:L:49:ASN:H	2:L:49:ASN:HD22	1.20	0.87
2:D:9:HIS:CD2	2:J:8:THR:HG23	2.09	0.86
2:B:138:LYS:O	2:B:141:VAL:HG13	1.73	0.86
2:F:67:LYS:HB2	2:F:68:PRO:HD3	1.57	0.86
2:B:142:GLU:OE1	2:B:146:ARG:NH2	2.07	0.86
2:H:158:MET:HE3	2:H:158:MET:HA	1.58	0.86
2:D:37:ILE:HD12	2:D:56:LEU:HD11	1.58	0.86
2:L:66:VAL:HG22	2:L:70:LEU:HD11	1.57	0.85
2:H:4:LEU:HD21	2:H:126:ARG:NH1	1.92	0.85
2:N:117:ALA:HB3	2:P:30:TYR:OH	1.77	0.85
1:K:58:VAL:HG22	1:K:63:LYS:HE3	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:HIS:HB3	2:H:61:LYS:HZ3	1.42	0.85
1:K:66:LEU:HD22	2:L:55:LEU:HD13	1.57	0.85
2:B:9:HIS:CD2	2:H:8:THR:HG23	2.12	0.84
2:L:49:ASN:H	2:L:49:ASN:ND2	1.75	0.84
2:L:2:VAL:O	2:L:3:LEU:HD23	1.78	0.84
2:J:2:VAL:HG12	2:J:128:LYS:NZ	1.92	0.84
2:J:65:TRP:O	2:J:68:PRO:HG3	1.77	0.84
1:G:43:SER:O	1:G:44:LYS:C	2.20	0.83
2:B:78:ILE:HD13	3:B:201:PX2:H8	1.61	0.83
2:J:66:VAL:O	2:J:69:PHE:N	2.11	0.83
2:L:67:LYS:HA	2:L:70:LEU:HD12	1.61	0.83
2:D:146:ARG:NH1	2:F:5:HIS:HA	1.94	0.83
1:G:61:GLY:O	1:G:64:PRO:HD2	1.79	0.83
2:B:14:ASP:OD1	2:B:17:SER:HB2	1.77	0.82
2:L:22:PHE:CD2	2:L:91:MET:HE1	2.14	0.82
1:I:4:ILE:O	1:I:5:MET:HE2	1.80	0.82
2:B:20:ARG:HD3	2:N:167:LEU:HD21	1.61	0.81
2:F:62:LEU:HD12	2:F:62:LEU:H	1.45	0.81
2:B:153:VAL:O	2:B:157:ARG:HG3	1.81	0.81
2:B:142:GLU:O	2:B:143:ASP:C	2.18	0.81
2:F:157:ARG:O	2:F:160:MET:HB2	1.81	0.81
2:N:94:TYR:OH	2:N:96:ARG:HD3	1.81	0.81
2:H:115:ASP:OD2	2:H:117:ALA:HB3	1.81	0.80
1:G:27:TRP:O	1:G:31:LYS:HB2	1.81	0.80
1:E:4:ILE:HG22	1:E:5:MET:H	1.46	0.79
1:E:6:SER:HB2	1:E:17:LYS:NZ	1.98	0.79
2:N:8:THR:HB	2:P:9:HIS:HD2	1.46	0.79
1:O:28:TYR:OH	2:P:84:VAL:HG11	1.82	0.79
2:H:101:THR:HG22	2:H:105:LYS:HD3	1.65	0.78
2:L:22:PHE:O	2:L:25:ARG:HG2	1.83	0.78
2:B:2:VAL:O	2:B:3:LEU:HD23	1.83	0.78
2:H:33:HIS:HB3	2:H:61:LYS:NZ	1.98	0.78
1:I:44:LYS:H	1:I:44:LYS:HD2	1.47	0.78
2:J:163:VAL:O	2:J:167:LEU:HB2	1.84	0.78
1:A:66:LEU:O	1:A:70:ARG:HG3	1.84	0.77
2:H:69:PHE:HA	2:H:71:ARG:CZ	2.15	0.77
2:L:91:MET:HE2	2:L:93:THR:HG22	1.65	0.77
2:L:2:VAL:HG22	2:L:128:LYS:HZ3	1.49	0.77
2:B:140:LYS:O	2:B:143:ASP:OD2	2.03	0.76
2:F:94:TYR:OH	2:F:107:GLU:HG2	1.85	0.76
2:B:102:GLY:O	2:B:132:GLY:CA	2.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:GLU:O	1:G:42:CYS:SG	2.44	0.76
2:N:160:MET:O	2:N:164:ILE:HG13	1.86	0.76
2:F:4:LEU:HA	2:F:127:VAL:O	1.86	0.76
2:F:3:LEU:O	2:F:4:LEU:HG	1.86	0.76
2:D:67:LYS:H	2:D:68:PRO:CD	1.76	0.75
2:D:70:LEU:O	2:D:70:LEU:HD22	1.87	0.75
2:B:138:LYS:HA	2:B:141:VAL:HG13	1.67	0.75
1:K:12:GLU:HG3	1:K:13:CYS:SG	2.26	0.75
1:A:4:ILE:O	1:A:5:MET:HE2	1.86	0.75
2:B:138:LYS:HA	2:B:141:VAL:CG1	2.17	0.74
2:B:113:GLN:HE21	2:B:113:GLN:CA	2.00	0.74
2:N:5:HIS:ND1	2:N:129:PHE:HE1	1.85	0.74
1:K:17:LYS:HB2	1:K:49:TYR:CE1	2.23	0.74
1:E:63:LYS:HB3	1:E:64:PRO:HD3	1.70	0.74
2:J:111:THR:HG22	2:J:124:ASP:HB3	1.68	0.74
2:H:84:VAL:HG22	2:H:91:MET:HE3	1.70	0.74
2:B:57:LYS:NZ	2:B:75:GLU:OE2	2.20	0.74
2:H:4:LEU:HD21	2:H:126:ARG:HH11	1.51	0.74
2:L:96:ARG:NH2	2:L:97:ASN:O	2.20	0.73
2:L:84:VAL:HG22	2:L:91:MET:HG3	1.69	0.73
2:F:168:GLU:O	2:F:169:GLU:HG3	1.88	0.73
2:F:25:ARG:NH2	2:F:26:TYR:CE2	2.56	0.72
2:B:25:ARG:NH1	2:B:80:GLU:OE1	2.22	0.72
2:B:10:ILE:HG12	2:B:122:ILE:HG12	1.70	0.72
2:J:49:ASN:OD1	2:J:85:ASN:HA	1.90	0.72
1:G:39:GLU:O	1:G:41:GLU:HG3	1.89	0.72
2:L:69:PHE:CD1	2:L:70:LEU:N	2.55	0.72
2:J:68:PRO:HG2	2:J:69:PHE:H	1.54	0.71
2:J:43:ASN:O	2:J:50:LEU:HD12	1.90	0.71
2:D:146:ARG:HH12	2:F:5:HIS:HA	1.53	0.71
1:G:25:ASN:HB3	2:H:20:ARG:HH12	1.54	0.71
2:J:2:VAL:O	2:J:3:LEU:HD12	1.90	0.71
2:L:15:PHE:CD1	2:L:89:SER:HB3	2.25	0.71
2:D:62:LEU:HB2	2:D:63:PRO:HD2	1.73	0.71
2:B:113:GLN:HE21	2:B:114:PHE:N	1.88	0.71
2:B:94:TYR:OH	2:B:96:ARG:HG2	1.90	0.70
2:F:80:GLU:CA	2:F:95:THR:HG22	2.21	0.70
2:B:138:LYS:C	2:B:141:VAL:HG13	2.17	0.70
1:K:5:MET:HE2	1:K:5:MET:HA	1.74	0.70
2:L:14:ASP:HA	2:L:114:PHE:HE2	1.55	0.70
2:J:70:LEU:O	2:J:72:GLY:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:ILE:HD12	2:H:56:LEU:HD11	1.73	0.70
2:H:146:ARG:HA	2:P:5:HIS:NE2	2.06	0.70
2:F:25:ARG:HD2	2:F:26:TYR:CZ	2.27	0.69
2:H:111:THR:O	2:H:123:ALA:HA	1.92	0.69
2:L:49:ASN:ND2	2:L:49:ASN:N	2.40	0.69
2:B:138:LYS:CA	2:B:141:VAL:HG13	2.22	0.69
1:I:46:TRP:O	1:I:50:THR:HG22	1.92	0.69
2:J:164:ILE:HD11	2:L:18:VAL:HA	1.73	0.69
1:E:61:GLY:O	1:E:64:PRO:HD2	1.92	0.69
2:H:2:VAL:O	2:H:3:LEU:HG	1.93	0.69
2:D:67:LYS:CB	2:D:68:PRO:HD3	2.21	0.68
2:J:68:PRO:HG2	2:J:69:PHE:N	2.08	0.68
1:K:63:LYS:N	1:K:64:PRO:HD2	2.08	0.68
2:D:13:THR:CG2	2:D:17:SER:HB3	2.23	0.68
1:K:58:VAL:HG22	1:K:63:LYS:CE	2.23	0.68
1:E:57:LEU:O	1:E:60:GLN:HB2	1.94	0.68
2:D:10:ILE:HD12	2:D:10:ILE:H	1.58	0.68
2:B:95:THR:HG23	2:B:108:GLU:HB3	1.76	0.68
2:B:140:LYS:O	2:B:143:ASP:OD1	2.12	0.68
2:J:154:LYS:HG2	2:J:158:MET:HE2	1.76	0.68
2:J:66:VAL:C	2:J:68:PRO:CD	2.67	0.68
2:L:2:VAL:HG22	2:L:128:LYS:NZ	2.08	0.68
1:K:58:VAL:HG13	1:K:63:LYS:HD2	1.75	0.68
2:L:15:PHE:H	2:L:114:PHE:HD2	1.41	0.68
2:P:131:SER:O	2:P:133:PHE:N	2.27	0.67
2:P:94:TYR:OH	2:P:96:ARG:HD3	1.94	0.67
2:F:162:PHE:CE1	2:F:166:LYS:HE3	2.29	0.67
1:G:43:SER:O	1:G:46:TRP:N	2.27	0.67
2:J:75:GLU:O	2:J:76:THR:OG1	2.10	0.67
2:P:3:LEU:O	2:P:4:LEU:HB3	1.93	0.67
2:B:143:ASP:HA	2:B:146:ARG:CD	2.25	0.67
2:F:122:ILE:HG12	2:J:158:MET:HG2	1.77	0.66
2:L:50:LEU:HD12	2:L:51:ARG:O	1.96	0.66
2:D:101:THR:HA	2:D:104:MET:O	1.95	0.66
2:J:101:THR:HG22	2:J:105:LYS:HD2	1.76	0.66
2:D:2:VAL:C	2:D:3:LEU:HD12	2.20	0.66
2:F:58:LYS:HG3	2:F:78:ILE:HD12	1.78	0.66
2:J:39:THR:HA	2:J:54:ARG:HG2	1.77	0.66
2:P:2:VAL:HA	2:P:129:PHE:O	1.96	0.66
2:B:113:GLN:HE21	2:B:113:GLN:HA	1.60	0.66
1:K:29:SER:HA	1:K:33:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:65:TRP:O	2:J:68:PRO:CG	2.44	0.66
2:L:1:MET:HE2	2:L:1:MET:HA	1.77	0.66
2:L:26:TYR:CE1	2:L:34:VAL:HG21	2.31	0.66
2:B:67:LYS:N	2:B:68:PRO:HD2	2.10	0.66
2:L:70:LEU:HB3	2:L:72:GLY:O	1.96	0.66
2:F:85:ASN:HB3	2:F:90:THR:HG22	1.77	0.66
1:K:16:LEU:HD13	1:K:48:ALA:O	1.96	0.66
1:K:17:LYS:O	1:K:20:TYR:N	2.29	0.66
2:J:3:LEU:O	2:J:4:LEU:HG	1.95	0.65
2:L:22:PHE:CE1	2:L:25:ARG:NH2	2.64	0.65
1:G:5:MET:HA	1:G:5:MET:HE2	1.77	0.65
1:G:6:SER:HB2	1:G:17:LYS:HZ3	1.60	0.65
1:I:25:ASN:HB3	2:J:20:ARG:HH22	1.61	0.65
2:B:39:THR:HA	2:B:54:ARG:HG2	1.76	0.65
2:J:63:PRO:O	2:J:64:THR:HG22	1.95	0.65
2:B:153:VAL:HG23	2:B:154:LYS:N	2.10	0.65
2:J:2:VAL:HG12	2:J:128:LYS:HZ1	1.59	0.65
2:L:67:LYS:CA	2:L:70:LEU:HD12	2.26	0.65
2:B:31:SER:N	2:B:32:PRO:CD	2.59	0.64
1:G:31:LYS:O	1:G:36:LYS:O	2.14	0.64
2:H:8:THR:CG2	2:N:157:ARG:HE	2.09	0.64
2:J:149:PHE:CZ	2:L:7:SER:HB2	2.24	0.64
2:P:157:ARG:HG2	2:P:157:ARG:HH11	1.62	0.64
2:D:147:THR:HG23	2:D:148:LYS:N	2.12	0.64
2:B:70:LEU:HD22	2:B:103:ILE:HD11	1.80	0.64
2:D:13:THR:HG22	2:D:17:SER:HB3	1.79	0.64
2:D:25:ARG:HA	2:F:163:VAL:HG21	1.79	0.64
1:G:40:ASN:OD1	1:G:41:GLU:N	2.31	0.64
2:D:63:PRO:HB2	2:D:68:PRO:HD3	1.80	0.64
2:P:2:VAL:HG22	2:P:130:SER:CB	2.23	0.64
2:P:2:VAL:HG11	2:P:128:LYS:CG	2.26	0.64
1:G:14:THR:O	1:G:17:LYS:HB3	1.97	0.64
2:B:113:GLN:HE21	2:B:114:PHE:H	1.46	0.64
1:C:61:GLY:O	1:C:64:PRO:HD2	1.98	0.64
2:D:108:GLU:HG3	2:D:127:VAL:HG22	1.80	0.64
2:F:73:ILE:HD12	2:F:73:ILE:O	1.96	0.64
1:I:31:LYS:HB3	1:I:36:LYS:HB3	1.80	0.64
2:J:96:ARG:HG3	2:J:97:ASN:O	1.97	0.64
2:L:91:MET:HE2	2:L:93:THR:CG2	2.28	0.64
2:B:142:GLU:O	2:B:144:TRP:N	2.30	0.63
1:K:56:ALA:O	1:K:60:GLN:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:LEU:C	2:F:4:LEU:HG	2.23	0.63
2:F:157:ARG:HG2	2:F:157:ARG:HH11	1.63	0.63
2:J:4:LEU:HA	2:J:127:VAL:O	1.97	0.63
2:J:70:LEU:O	2:J:70:LEU:HD12	1.96	0.63
2:L:31:SER:HA	2:L:33:HIS:CE1	2.33	0.63
2:J:62:LEU:O	2:J:64:THR:N	2.32	0.63
2:J:96:ARG:HA	2:J:106:VAL:O	1.99	0.63
2:H:30:TYR:CE1	2:P:158:MET:HE3	2.32	0.63
1:E:6:SER:HB2	1:E:17:LYS:HZ1	1.63	0.63
2:N:5:HIS:HB2	2:N:127:VAL:HB	1.81	0.63
1:K:6:SER:HB3	1:K:17:LYS:HZ1	1.63	0.63
2:L:14:ASP:OD2	2:L:16:ALA:HB3	1.99	0.63
2:N:153:VAL:O	2:N:157:ARG:CG	2.47	0.62
2:N:166:LYS:C	2:N:168:GLU:H	2.06	0.62
2:P:142:GLU:HG3	2:P:143:ASP:N	2.13	0.62
1:K:10:ALA:O	1:K:12:GLU:N	2.32	0.62
1:K:19:LYS:HB3	1:K:45:GLN:HG2	1.80	0.62
2:D:50:LEU:O	2:D:83:VAL:HA	1.99	0.62
2:L:35:LEU:HB2	2:L:57:LYS:HD3	1.81	0.62
2:L:68:PRO:HG2	2:L:69:PHE:H	1.62	0.62
2:L:94:TYR:OH	2:L:96:ARG:HD3	1.99	0.62
1:E:6:SER:HB2	1:E:17:LYS:HZ3	1.64	0.62
1:G:4:ILE:HG22	1:G:5:MET:H	1.65	0.62
2:L:161:ALA:O	2:L:164:ILE:HB	1.99	0.62
1:K:28:TYR:CZ	1:K:33:LEU:HD21	2.35	0.62
2:P:51:ARG:NE	2:P:83:VAL:HG22	2.15	0.62
2:F:97:ASN:HB3	3:F:201:PX2:H17	1.81	0.62
2:H:70:LEU:HD22	2:H:74:THR:OG1	1.99	0.62
2:F:67:LYS:CB	2:F:68:PRO:HD3	2.29	0.62
2:L:154:LYS:HG2	2:L:158:MET:HE2	1.81	0.62
2:N:73:ILE:HD12	2:N:74:THR:H	1.64	0.62
2:N:153:VAL:O	2:N:157:ARG:HG3	1.99	0.62
2:P:153:VAL:O	2:P:156:SER:HB3	1.98	0.62
2:P:165:GLN:HG2	2:P:166:LYS:N	2.15	0.62
2:B:67:LYS:N	2:B:68:PRO:CD	2.63	0.61
2:B:84:VAL:HG22	2:B:91:MET:HB2	1.82	0.61
2:B:148:LYS:O	2:B:148:LYS:HD3	2.00	0.61
2:D:30:TYR:HD2	2:F:159:GLY:HA2	1.64	0.61
2:H:161:ALA:HB3	2:N:118:THR:HG21	1.81	0.61
2:L:94:TYR:CD1	2:L:94:TYR:C	2.78	0.61
1:I:25:ASN:HB3	2:J:20:ARG:NH2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45:ASP:OD2	2:F:51:ARG:HD3	2.00	0.61
2:H:8:THR:HG21	2:N:157:ARG:HE	1.65	0.61
1:K:54:ASN:O	1:K:58:VAL:HG23	2.00	0.61
2:N:134:ASN:O	2:N:137:ILE:HB	2.00	0.61
2:D:63:PRO:HB2	2:D:68:PRO:CD	2.30	0.61
2:D:133:PHE:HA	2:H:68:PRO:HG2	1.82	0.61
2:F:4:LEU:N	2:F:4:LEU:HD12	2.14	0.61
2:J:70:LEU:HD12	2:J:70:LEU:C	2.24	0.61
2:N:3:LEU:HD13	2:N:3:LEU:N	2.15	0.61
2:B:68:PRO:HG2	2:B:69:PHE:H	1.66	0.61
2:B:76:THR:OG1	3:B:201:PX2:H44	2.01	0.61
1:K:32:PHE:CZ	2:L:86:PRO:HG2	2.35	0.61
2:J:67:LYS:N	2:J:68:PRO:HD2	2.16	0.61
2:P:129:PHE:N	2:P:129:PHE:CD1	2.67	0.61
1:A:46:TRP:O	1:A:50:THR:HG22	2.01	0.61
2:D:110:THR:OG1	2:D:125:SER:HB3	2.01	0.61
2:J:66:VAL:C	2:J:68:PRO:HD2	2.26	0.61
2:B:70:LEU:CD2	2:B:103:ILE:HD11	2.31	0.61
1:E:39:GLU:O	1:E:40:ASN:C	2.43	0.60
2:F:25:ARG:NH2	2:F:26:TYR:HE2	2.00	0.60
2:J:3:LEU:C	2:J:4:LEU:HD12	2.26	0.60
2:L:2:VAL:C	2:L:3:LEU:HD23	2.26	0.60
2:L:137:ILE:O	2:L:141:VAL:HG23	2.00	0.60
2:P:13:THR:CG2	2:P:17:SER:HB2	2.32	0.60
2:B:157:ARG:HH11	2:B:157:ARG:HG2	1.66	0.60
3:B:201:PX2:H45	3:B:201:PX2:H22	1.82	0.60
2:B:129:PHE:C	2:B:130:SER:OG	2.36	0.60
2:H:62:LEU:O	2:H:63:PRO:C	2.45	0.60
1:K:28:TYR:OH	2:L:84:VAL:HG11	2.01	0.60
2:H:13:THR:HG22	2:H:14:ASP:H	1.67	0.60
2:H:82:SER:HB3	2:H:93:THR:HG22	1.84	0.60
1:K:49:TYR:O	1:K:53:VAL:HG23	2.01	0.60
2:D:144:TRP:O	2:D:147:THR:HG22	2.01	0.60
1:I:36:LYS:HB2	1:I:36:LYS:HZ3	1.65	0.60
2:D:18:VAL:HA	2:F:164:ILE:HD11	1.82	0.60
2:D:37:ILE:CD1	2:D:56:LEU:HD11	2.30	0.60
2:D:96:ARG:HH21	2:D:96:ARG:HG3	1.66	0.60
1:E:14:THR:O	1:E:17:LYS:HB3	2.02	0.60
2:B:143:ASP:HA	2:B:146:ARG:CG	2.32	0.59
2:F:28:ASN:HB2	2:F:29:PRO:HD2	1.83	0.59
2:F:149:PHE:HA	2:F:152:ASN:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:97:ASN:C	2:J:97:ASN:HD22	2.10	0.59
2:B:45:ASP:HB3	2:B:51:ARG:NH2	2.17	0.59
2:F:104:MET:HB2	2:F:129:PHE:HE1	1.67	0.59
2:N:166:LYS:HG3	2:N:167:LEU:N	2.16	0.59
2:D:9:HIS:CD2	2:F:157:ARG:HD3	2.38	0.59
2:H:31:SER:HA	2:H:33:HIS:CE1	2.38	0.59
2:B:137:ILE:C	2:B:141:VAL:HG12	2.28	0.59
2:J:148:LYS:O	2:J:149:PHE:C	2.45	0.59
2:L:55:LEU:HD21	2:L:77:TRP:CE3	2.38	0.59
2:N:137:ILE:HG22	2:N:138:LYS:N	2.18	0.59
2:B:142:GLU:O	2:B:145:SER:N	2.35	0.59
2:J:3:LEU:HB3	2:J:129:PHE:CD2	2.38	0.59
2:N:168:GLU:O	2:N:169:GLU:HG3	2.03	0.59
2:D:9:HIS:CD2	2:J:8:THR:O	2.56	0.59
2:B:137:ILE:O	2:B:141:VAL:HG12	2.02	0.58
2:J:25:ARG:HA	2:L:163:VAL:HG21	1.85	0.58
1:K:12:GLU:OE1	1:K:56:ALA:HB2	2.03	0.58
2:J:66:VAL:C	2:J:68:PRO:HG2	2.27	0.58
1:C:46:TRP:O	1:C:50:THR:HG22	2.04	0.58
1:G:39:GLU:N	1:G:39:GLU:OE1	2.36	0.58
1:I:39:GLU:OE1	1:I:39:GLU:N	2.36	0.58
1:K:24:PHE:C	1:K:26:GLU:H	2.10	0.58
2:N:95:THR:OG1	2:N:108:GLU:HB3	2.04	0.58
2:F:26:TYR:CE1	2:F:34:VAL:HG21	2.39	0.58
2:B:143:ASP:HA	2:B:146:ARG:HG3	1.85	0.58
2:F:164:ILE:O	2:F:168:GLU:HG3	2.02	0.58
2:H:4:LEU:C	2:H:5:HIS:ND1	2.62	0.58
2:L:14:ASP:HA	2:L:114:PHE:CE2	2.36	0.58
2:L:39:THR:O	2:L:40:ILE:HD12	2.04	0.58
2:N:3:LEU:C	2:N:3:LEU:HD22	2.28	0.58
2:N:59:SER:HA	2:N:75:GLU:OE2	2.03	0.58
2:L:129:PHE:CD1	2:L:129:PHE:C	2.81	0.58
2:N:8:THR:HB	2:P:9:HIS:CD2	2.35	0.58
2:H:62:LEU:O	2:H:62:LEU:HD13	2.04	0.58
2:J:155:LYS:HA	2:J:158:MET:HE3	1.86	0.58
2:B:151:GLU:O	2:B:155:LYS:HB2	2.04	0.58
2:F:3:LEU:C	2:F:4:LEU:CG	2.73	0.58
2:F:22:PHE:CD2	2:F:91:MET:HE1	2.39	0.58
2:J:66:VAL:O	2:J:68:PRO:CG	2.51	0.58
2:B:29:PRO:HG2	2:N:162:PHE:CE2	2.39	0.57
2:B:37:ILE:HD12	2:B:56:LEU:CD2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:113:GLN:HE22	2:J:154:LYS:NZ	2.01	0.57
2:L:153:VAL:O	2:L:154:LYS:C	2.46	0.57
2:H:94:TYR:OH	2:H:96:ARG:HD3	2.03	0.57
2:H:2:VAL:O	2:H:3:LEU:CG	2.52	0.57
2:J:3:LEU:HB3	2:J:129:PHE:HD2	1.69	0.57
2:H:88:ASN:OD1	2:H:90:THR:HB	2.04	0.57
1:C:17:LYS:HB2	1:C:49:TYR:CE1	2.39	0.57
2:D:131:SER:HB3	2:D:134:ASN:HB3	1.86	0.57
1:I:48:ALA:O	1:I:51:THR:HB	2.03	0.57
1:I:66:LEU:C	1:I:68:GLU:H	2.12	0.57
2:P:4:LEU:CB	2:P:127:VAL:O	2.49	0.57
2:B:9:HIS:HB2	2:N:157:ARG:NE	2.20	0.57
2:D:10:ILE:HG23	2:D:122:ILE:HG12	1.87	0.57
1:O:47:TYR:HA	1:O:50:THR:HG22	1.87	0.57
1:K:6:SER:HB3	1:K:17:LYS:NZ	2.19	0.57
2:N:8:THR:CB	2:P:9:HIS:HD2	2.16	0.57
2:N:133:PHE:CD1	2:N:133:PHE:C	2.82	0.57
1:G:58:VAL:C	1:G:60:GLN:H	2.13	0.57
2:F:10:ILE:HG12	2:F:122:ILE:HG13	1.86	0.57
2:H:69:PHE:CE2	2:H:74:THR:HG23	2.39	0.57
1:K:58:VAL:HG22	1:K:63:LYS:CD	2.34	0.57
1:A:23:CYS:SG	1:A:24:PHE:N	2.75	0.56
2:H:42:ARG:HA	2:H:51:ARG:O	2.05	0.56
1:I:28:TYR:OH	2:J:19:SER:HB2	2.06	0.56
1:K:17:LYS:O	1:K:18:THR:C	2.46	0.56
2:N:3:LEU:N	2:N:129:PHE:O	2.38	0.56
2:P:4:LEU:C	2:P:4:LEU:HD12	2.29	0.56
2:F:85:ASN:OD1	2:F:87:ALA:HB3	2.05	0.56
2:P:2:VAL:CG1	2:P:128:LYS:CG	2.82	0.56
1:G:40:ASN:C	1:G:41:GLU:HG3	2.29	0.56
2:H:84:VAL:HG22	2:H:91:MET:HE1	1.87	0.56
2:L:73:ILE:HD12	2:L:73:ILE:N	2.13	0.56
2:D:51:ARG:CD	2:D:83:VAL:HG22	2.36	0.56
1:I:16:LEU:H	1:I:16:LEU:HD23	1.71	0.56
1:I:36:LYS:HA	1:I:36:LYS:HZ2	1.68	0.56
2:F:10:ILE:HG23	2:F:122:ILE:HD12	1.88	0.56
1:E:63:LYS:HE2	1:E:67:ASP:OD2	2.04	0.56
1:I:15:ASP:HB2	1:I:16:LEU:HD23	1.87	0.56
1:I:45:GLN:OE1	1:I:45:GLN:N	2.39	0.56
1:I:44:LYS:HD2	1:I:44:LYS:N	2.20	0.56
2:J:10:ILE:HG23	2:J:122:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:69:PHE:O	2:J:70:LEU:HG	2.06	0.56
2:P:13:THR:HG22	2:P:17:SER:HB2	1.87	0.56
2:P:105:LYS:O	2:P:129:PHE:HA	2.05	0.56
2:D:147:THR:CG2	2:D:148:LYS:N	2.69	0.56
2:F:104:MET:HB2	2:F:129:PHE:CE1	2.41	0.56
2:J:5:HIS:HD2	2:L:150:ASP:OD1	1.89	0.56
2:J:160:MET:HE1	2:L:112:TYR:CE1	2.41	0.56
1:M:63:LYS:HB3	1:M:64:PRO:HD3	1.88	0.56
2:F:44:VAL:HA	2:F:49:ASN:O	2.06	0.55
2:J:42:ARG:HG3	2:J:42:ARG:HH11	1.70	0.55
2:J:163:VAL:HG13	2:J:167:LEU:HD22	1.88	0.55
2:B:1:MET:O	2:B:130:SER:HA	2.07	0.55
1:E:60:GLN:CB	1:E:62:ILE:HG22	2.27	0.55
2:F:105:LYS:HE2	2:F:107:GLU:CD	2.32	0.55
2:J:68:PRO:C	2:J:70:LEU:H	2.12	0.55
1:K:10:ALA:C	1:K:12:GLU:H	2.13	0.55
1:K:43:SER:HA	1:K:46:TRP:HB3	1.87	0.55
2:D:4:LEU:HA	2:D:127:VAL:O	2.06	0.55
1:I:38:VAL:HG13	1:I:39:GLU:N	2.11	0.55
2:J:42:ARG:O	2:J:43:ASN:HB2	2.06	0.55
1:K:28:TYR:CE2	1:K:33:LEU:HD11	2.41	0.55
1:A:47:TYR:HA	1:A:50:THR:CG2	2.36	0.55
2:F:85:ASN:OD1	2:F:88:ASN:OD1	2.23	0.55
2:F:157:ARG:HD2	2:J:8:THR:HG21	1.89	0.55
2:B:153:VAL:HG23	2:B:154:LYS:H	1.72	0.55
2:F:118:THR:HA	2:J:165:GLN:HE22	1.72	0.55
2:J:111:THR:HG22	2:J:124:ASP:CB	2.35	0.55
1:I:69:ALA:C	1:I:71:GLU:H	2.15	0.55
2:N:5:HIS:ND1	2:N:129:PHE:CE1	2.69	0.55
2:D:85:ASN:OD1	2:D:87:ALA:HB3	2.07	0.55
2:D:164:ILE:HG21	2:F:13:THR:HG21	1.89	0.55
2:J:130:SER:O	2:J:131:SER:HB2	2.05	0.55
2:H:62:LEU:N	2:H:63:PRO:HD2	2.21	0.54
2:P:2:VAL:HG11	2:P:128:LYS:HG3	1.88	0.54
2:P:103:ILE:O	2:P:131:SER:HB2	2.07	0.54
2:B:76:THR:HG23	2:B:99:ASP:OD1	2.08	0.54
2:H:91:MET:HG2	2:H:112:TYR:HD2	1.72	0.54
2:J:163:VAL:HG21	2:L:25:ARG:CA	2.25	0.54
2:L:35:LEU:HB2	2:L:57:LYS:CD	2.36	0.54
1:E:21:ASP:O	1:E:22:SER:C	2.51	0.54
2:J:69:PHE:O	2:J:71:ARG:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6:SER:HB3	2:N:27:PRO:HD3	1.87	0.54
2:N:13:THR:HG22	2:N:17:SER:HB2	1.90	0.54
2:D:9:HIS:CE1	2:D:11:PHE:CE1	2.95	0.54
1:K:63:LYS:N	1:K:64:PRO:CD	2.70	0.54
2:H:122:ILE:HG23	2:N:158:MET:HE3	1.89	0.54
1:I:16:LEU:HD23	1:I:16:LEU:N	2.23	0.54
2:J:28:ASN:HB2	2:J:29:PRO:HD2	1.90	0.54
2:B:153:VAL:HG23	2:B:154:LYS:HE3	1.89	0.54
1:E:53:VAL:O	1:E:54:ASN:C	2.51	0.54
2:J:66:VAL:C	2:J:68:PRO:CG	2.81	0.54
1:A:16:LEU:HD13	1:A:48:ALA:HB1	1.88	0.54
1:A:42:CYS:O	1:A:43:SER:C	2.51	0.54
2:N:73:ILE:HG13	2:N:74:THR:N	2.21	0.54
2:J:46:GLN:O	2:J:47:GLU:HG3	2.08	0.54
1:K:58:VAL:CG2	1:K:63:LYS:HE3	2.34	0.54
2:B:113:GLN:NE2	2:B:114:PHE:H	2.05	0.54
2:D:33:HIS:CD2	2:D:33:HIS:H	2.25	0.54
2:H:161:ALA:HB3	2:N:118:THR:CG2	2.37	0.54
2:J:25:ARG:NH2	2:J:26:TYR:CE2	2.76	0.54
2:N:73:ILE:CD1	2:N:74:THR:H	2.19	0.54
2:F:100:HIS:C	2:F:102:GLY:H	2.16	0.53
2:F:139:SER:O	2:F:140:LYS:C	2.51	0.53
2:B:96:ARG:HB2	2:B:106:VAL:O	2.07	0.53
2:L:57:LYS:HB2	2:L:77:TRP:CZ3	2.43	0.53
2:B:31:SER:N	2:B:32:PRO:HD2	2.22	0.53
2:D:3:LEU:HD12	2:D:3:LEU:N	2.23	0.53
2:J:103:ILE:O	2:J:103:ILE:HG22	2.07	0.53
2:J:128:LYS:O	2:J:128:LYS:HD3	2.09	0.53
1:I:30:GLU:O	1:I:34:LYS:HB2	2.08	0.53
1:I:66:LEU:O	1:I:68:GLU:N	2.41	0.53
2:L:6:LYS:HG2	2:L:126:ARG:CG	2.37	0.53
2:P:2:VAL:CG1	2:P:128:LYS:HG2	2.38	0.53
2:D:7:SER:HB3	2:J:6:LYS:HD2	1.91	0.53
1:M:66:LEU:O	1:M:70:ARG:HG3	2.08	0.53
1:O:24:PHE:CE1	2:P:42:ARG:HD3	2.44	0.53
1:E:53:VAL:O	1:E:57:LEU:N	2.39	0.53
2:J:42:ARG:HG3	2:J:42:ARG:NH1	2.23	0.53
2:B:26:TYR:CE1	2:B:34:VAL:HG21	2.44	0.53
2:B:78:ILE:HG23	2:B:96:ARG:O	2.09	0.53
2:B:94:TYR:CZ	2:B:96:ARG:HG2	2.43	0.53
2:D:99:ASP:O	2:D:100:HIS:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:85:ASN:OD1	2:H:87:ALA:HB3	2.08	0.53
2:D:102:GLY:H	2:H:71:ARG:NH2	2.07	0.53
2:H:67:LYS:N	2:H:68:PRO:CD	2.71	0.53
2:H:158:MET:HA	2:H:158:MET:CE	2.34	0.53
2:B:96:ARG:HD2	2:B:97:ASN:O	2.09	0.53
2:F:79:ILE:CG2	2:F:98:LEU:HD23	2.39	0.53
2:F:113:GLN:NE2	2:J:154:LYS:NZ	2.57	0.53
2:H:40:ILE:O	2:H:41:SER:HB3	2.09	0.53
2:J:43:ASN:OD1	2:J:44:VAL:N	2.42	0.53
1:C:37:SER:O	1:C:38:VAL:HG23	2.08	0.52
2:D:70:LEU:H	2:D:70:LEU:CD1	2.22	0.52
1:I:31:LYS:C	1:I:36:LYS:HB3	2.35	0.52
2:L:114:PHE:HE1	2:L:116:SER:HA	1.74	0.52
1:C:54:ASN:O	1:C:55:ALA:C	2.52	0.52
2:D:73:ILE:O	2:D:73:ILE:HG13	2.07	0.52
1:E:40:ASN:C	1:E:42:CYS:H	2.17	0.52
2:F:8:THR:HA	2:F:123:ALA:O	2.09	0.52
2:H:49:ASN:OD1	2:H:85:ASN:HA	2.09	0.52
2:B:56:LEU:N	2:B:56:LEU:HD12	2.24	0.52
2:H:129:PHE:CD1	2:H:130:SER:N	2.77	0.52
2:J:111:THR:HG23	2:J:111:THR:O	2.08	0.52
2:D:33:HIS:CD2	2:D:33:HIS:N	2.78	0.52
1:E:6:SER:CB	1:E:17:LYS:NZ	2.72	0.52
2:H:4:LEU:O	2:H:5:HIS:ND1	2.43	0.52
2:J:42:ARG:NH1	2:J:52:THR:HG21	2.24	0.52
2:J:67:LYS:N	2:J:68:PRO:CD	2.71	0.52
2:L:96:ARG:HH21	2:L:96:ARG:HG3	1.73	0.52
2:B:58:LYS:NZ	3:B:201:PX2:H2	2.25	0.52
2:J:10:ILE:HG12	2:J:122:ILE:CD1	2.40	0.52
2:N:73:ILE:O	2:N:74:THR:HG23	2.09	0.52
2:P:76:THR:HG23	2:P:99:ASP:OD1	2.10	0.52
2:F:99:ASP:O	2:F:100:HIS:HB2	2.08	0.52
1:G:43:SER:C	1:G:45:GLN:N	2.65	0.52
1:I:9:PHE:CZ	1:I:57:LEU:HD23	2.44	0.52
2:B:138:LYS:CA	2:B:141:VAL:CG1	2.85	0.52
2:F:94:TYR:OH	2:F:96:ARG:HD3	2.10	0.52
2:F:157:ARG:CD	2:J:8:THR:HG21	2.39	0.52
2:L:84:VAL:O	2:L:86:PRO:HD3	2.10	0.52
1:G:25:ASN:HB3	2:H:20:ARG:NH1	2.21	0.52
1:K:24:PHE:C	1:K:26:GLU:N	2.67	0.52
2:L:15:PHE:N	2:L:114:PHE:HD2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:137:ILE:O	2:N:138:LYS:C	2.52	0.52
2:D:22:PHE:O	2:D:25:ARG:HB3	2.10	0.51
2:L:45:ASP:HB3	2:L:47:GLU:OE1	2.10	0.51
2:D:57:LYS:HG3	2:D:77:TRP:CZ3	2.45	0.51
2:N:13:THR:CG2	2:N:17:SER:HB2	2.41	0.51
2:B:64:THR:HA	2:B:67:LYS:HD3	1.92	0.51
2:H:111:THR:O	2:H:111:THR:HG22	2.10	0.51
2:H:158:MET:HE2	2:N:118:THR:HG21	1.93	0.51
1:M:47:TYR:HA	1:M:50:THR:HG22	1.92	0.51
1:O:74:PRO:HB2	1:O:75:PHE:CE1	2.45	0.51
1:A:63:LYS:N	1:A:64:PRO:HD2	2.25	0.51
2:F:4:LEU:CA	2:F:127:VAL:O	2.58	0.51
2:H:26:TYR:CE1	2:H:34:VAL:HG21	2.46	0.51
2:J:22:PHE:CE2	2:J:93:THR:HG21	2.45	0.51
2:L:149:PHE:HA	2:L:152:ASN:HD22	1.76	0.51
2:D:2:VAL:HA	2:D:129:PHE:O	2.10	0.51
2:D:137:ILE:O	2:D:141:VAL:HG23	2.10	0.51
1:G:6:SER:HB2	1:G:17:LYS:NZ	2.25	0.51
2:H:25:ARG:NH2	2:H:26:TYR:CE2	2.79	0.51
1:I:24:PHE:CE1	2:J:42:ARG:HD3	2.45	0.51
2:D:164:ILE:O	2:D:168:GLU:HG3	2.11	0.51
2:N:73:ILE:CG1	2:N:74:THR:N	2.73	0.51
2:B:15:PHE:HB2	2:B:114:PHE:HB2	1.91	0.51
2:L:6:LYS:HG2	2:L:126:ARG:HG2	1.92	0.51
2:N:164:ILE:O	2:N:168:GLU:HG3	2.11	0.51
2:B:28:ASN:HB2	2:B:29:PRO:HD2	1.93	0.51
2:B:113:GLN:HE21	2:B:113:GLN:C	2.19	0.51
2:H:112:TYR:CD1	2:H:123:ALA:HB2	2.46	0.51
2:L:13:THR:HG22	2:L:14:ASP:H	1.76	0.51
1:O:33:LEU:HD23	2:P:86:PRO:HB3	1.93	0.51
1:E:6:SER:CB	1:E:17:LYS:HZ1	2.23	0.51
2:F:76:THR:HG21	3:F:201:PX2:H42	1.91	0.51
1:K:10:ALA:C	1:K:12:GLU:N	2.69	0.51
1:G:41:GLU:C	1:G:42:CYS:SG	2.94	0.50
2:J:2:VAL:HG12	2:J:128:LYS:HZ2	1.74	0.50
2:J:35:LEU:HD11	2:J:59:SER:HB3	1.93	0.50
2:L:31:SER:O	2:L:34:VAL:HG23	2.11	0.50
2:N:89:SER:HB3	2:N:114:PHE:HB3	1.93	0.50
2:B:113:GLN:NE2	2:B:114:PHE:N	2.57	0.50
2:H:60:GLY:H	2:H:75:GLU:HA	1.76	0.50
2:H:129:PHE:CD1	2:H:129:PHE:C	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:164:ILE:HG13	2:L:21:ALA:HB2	1.93	0.50
1:K:18:THR:O	1:K:21:ASP:HB2	2.11	0.50
2:L:18:VAL:O	2:L:21:ALA:HB3	2.11	0.50
1:O:20:TYR:OH	2:P:42:ARG:HD2	2.11	0.50
1:G:13:CYS:O	1:G:14:THR:C	2.54	0.50
2:H:10:ILE:HG12	2:H:122:ILE:HG22	1.94	0.50
2:H:11:PHE:HE2	2:H:112:TYR:HE1	1.59	0.50
1:C:38:VAL:HG13	1:C:39:GLU:N	2.25	0.50
1:E:65:ALA:O	1:E:68:GLU:HB3	2.11	0.50
1:I:7:ALA:HA	1:I:14:THR:HG23	1.92	0.50
2:J:105:LYS:HB3	2:J:130:SER:HB2	1.94	0.50
2:N:3:LEU:N	2:N:3:LEU:CD1	2.74	0.50
1:A:66:LEU:O	1:A:66:LEU:HD12	2.11	0.50
2:B:113:GLN:HA	2:B:113:GLN:NE2	2.27	0.50
1:K:12:GLU:CD	1:K:56:ALA:HB2	2.37	0.50
2:L:13:THR:CG2	2:L:17:SER:HB2	2.42	0.50
2:L:69:PHE:HD1	2:L:70:LEU:H	1.50	0.50
2:P:1:MET:O	2:P:130:SER:HB2	2.11	0.50
2:P:139:SER:O	2:P:143:ASP:HB2	2.12	0.50
1:E:46:TRP:O	1:E:47:TYR:C	2.54	0.50
2:F:100:HIS:C	2:F:102:GLY:N	2.68	0.50
2:J:90:THR:CG2	2:J:92:LYS:HE2	2.41	0.50
2:L:25:ARG:O	2:L:27:PRO:O	2.30	0.50
2:N:13:THR:HG22	2:N:14:ASP:N	2.27	0.50
2:N:166:LYS:C	2:N:168:GLU:N	2.68	0.50
2:B:57:LYS:HD2	2:B:77:TRP:CD2	2.47	0.50
1:C:23:CYS:SG	1:C:45:GLN:NE2	2.85	0.50
2:D:25:ARG:NH1	2:D:80:GLU:OE1	2.42	0.50
2:L:15:PHE:HB2	2:L:114:PHE:HB2	1.94	0.50
2:L:28:ASN:OD1	2:L:28:ASN:C	2.55	0.50
1:A:4:ILE:HG22	1:A:5:MET:H	1.77	0.50
2:F:99:ASP:OD1	2:F:99:ASP:N	2.44	0.50
1:G:63:LYS:HG2	1:G:67:ASP:OD2	2.12	0.50
2:J:14:ASP:OD1	2:J:16:ALA:N	2.42	0.50
1:E:41:GLU:OE2	1:E:41:GLU:N	2.45	0.50
2:F:130:SER:O	2:F:131:SER:HB2	2.12	0.50
2:F:157:ARG:HE	2:J:8:THR:HG21	1.77	0.50
2:H:101:THR:CG2	2:H:105:LYS:HD3	2.40	0.50
2:J:10:ILE:HG12	2:J:122:ILE:HD12	1.94	0.50
2:L:66:VAL:O	2:L:67:LYS:CB	2.60	0.50
1:A:47:TYR:HA	1:A:50:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:HIS:NE2	2:H:10:ILE:HG13	2.27	0.49
2:H:65:TRP:CD1	2:H:65:TRP:C	2.90	0.49
2:H:149:PHE:CD1	2:H:149:PHE:C	2.89	0.49
1:I:25:ASN:O	1:I:29:SER:HB2	2.12	0.49
1:I:27:TRP:CZ2	1:I:32:PHE:HB2	2.46	0.49
2:L:13:THR:HG21	2:L:17:SER:HB2	1.93	0.49
2:L:94:TYR:C	2:L:94:TYR:HD1	2.19	0.49
1:A:39:GLU:O	1:A:40:ASN:C	2.54	0.49
2:B:153:VAL:CG2	2:B:154:LYS:N	2.75	0.49
2:D:168:GLU:O	2:D:169:GLU:HG3	2.12	0.49
2:F:141:VAL:HG23	2:F:142:GLU:N	2.25	0.49
2:J:26:TYR:CE1	2:J:34:VAL:HG21	2.47	0.49
2:D:9:HIS:CG	2:F:157:ARG:HD3	2.47	0.49
1:C:38:VAL:CG1	1:C:39:GLU:N	2.75	0.49
2:D:140:LYS:O	2:D:142:GLU:N	2.46	0.49
2:F:67:LYS:HB2	2:F:68:PRO:CD	2.38	0.49
2:J:159:GLY:HA2	2:L:30:TYR:HD2	1.78	0.49
2:L:43:ASN:C	2:L:43:ASN:OD1	2.55	0.49
1:C:16:LEU:HD13	1:C:48:ALA:HB1	1.94	0.49
1:C:24:PHE:CD1	1:C:24:PHE:C	2.91	0.49
3:F:201:PX2:H7	3:F:201:PX2:C17	2.43	0.49
1:I:26:GLU:O	1:I:27:TRP:C	2.56	0.49
1:K:75:PHE:O	1:K:76:GLU:C	2.55	0.49
2:L:13:THR:HG21	2:L:17:SER:CB	2.43	0.49
2:L:155:LYS:HA	2:L:158:MET:HE3	1.94	0.49
2:D:70:LEU:H	2:D:70:LEU:HD13	1.78	0.49
2:D:91:MET:HB3	2:D:112:TYR:HB2	1.94	0.49
2:F:157:ARG:NE	2:J:8:THR:HG21	2.28	0.49
1:M:6:SER:CA	2:N:27:PRO:HD3	2.43	0.49
2:P:133:PHE:CD1	2:P:134:ASN:N	2.80	0.49
2:J:9:HIS:CG	2:L:157:ARG:HD3	2.48	0.49
2:N:53:THR:HA	2:N:80:GLU:O	2.13	0.49
2:F:103:ILE:HG22	2:F:104:MET:HE3	1.95	0.49
2:N:110:THR:HA	2:N:124:ASP:O	2.12	0.49
2:P:42:ARG:HH21	2:P:52:THR:HG21	1.78	0.49
1:G:37:SER:HA	1:G:38:VAL:HG13	1.95	0.49
1:G:43:SER:HA	1:G:46:TRP:HB3	1.94	0.49
2:J:90:THR:HG23	2:J:92:LYS:HE2	1.95	0.49
2:B:83:VAL:O	2:B:91:MET:HA	2.13	0.49
2:B:111:THR:O	2:B:123:ALA:HA	2.13	0.49
2:D:3:LEU:O	2:D:4:LEU:CD2	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1:MET:O	2:L:2:VAL:CG2	2.53	0.49
1:A:15:ASP:O	1:A:16:LEU:C	2.56	0.48
2:F:45:ASP:OD2	2:F:49:ASN:HB2	2.13	0.48
2:F:99:ASP:O	2:F:100:HIS:CB	2.61	0.48
2:H:42:ARG:O	2:H:43:ASN:HB3	2.13	0.48
2:B:76:THR:HG22	2:B:77:TRP:O	2.13	0.48
2:H:10:ILE:HG23	2:H:122:ILE:HG22	1.94	0.48
1:I:9:PHE:CE2	1:I:57:LEU:HD23	2.47	0.48
1:I:44:LYS:H	1:I:44:LYS:CD	2.23	0.48
2:L:37:ILE:HD13	2:L:56:LEU:HG	1.95	0.48
2:L:45:ASP:HB2	2:L:49:ASN:O	2.13	0.48
1:A:27:TRP:CH2	1:A:32:PHE:HB2	2.48	0.48
1:A:40:ASN:C	1:A:42:CYS:H	2.21	0.48
2:F:68:PRO:C	2:F:70:LEU:H	2.21	0.48
2:N:115:ASP:OD2	2:P:30:TYR:OH	2.26	0.48
1:A:9:PHE:CE2	1:A:53:VAL:HG13	2.49	0.48
2:B:146:ARG:HA	2:N:5:HIS:NE2	2.28	0.48
2:D:3:LEU:O	2:D:4:LEU:HD13	2.13	0.48
2:D:111:THR:O	2:D:123:ALA:HA	2.14	0.48
2:F:100:HIS:O	2:F:102:GLY:N	2.46	0.48
2:P:51:ARG:HE	2:P:83:VAL:HG22	1.76	0.48
2:B:25:ARG:O	2:B:28:ASN:ND2	2.45	0.48
2:F:141:VAL:CG2	2:F:142:GLU:N	2.76	0.48
2:F:142:GLU:O	2:F:146:ARG:HG3	2.13	0.48
2:F:165:GLN:OE1	2:J:118:THR:HG22	2.13	0.48
2:J:66:VAL:C	2:J:68:PRO:N	2.71	0.48
2:J:131:SER:O	2:J:132:GLY:C	2.56	0.48
2:L:49:ASN:HB3	2:L:84:VAL:O	2.12	0.48
2:H:42:ARG:NH2	2:H:52:THR:HG21	2.27	0.48
2:H:62:LEU:HD13	2:H:62:LEU:C	2.39	0.48
1:I:25:ASN:HB3	2:J:20:ARG:NH1	2.29	0.48
1:E:37:SER:HB2	1:E:39:GLU:OE1	2.13	0.48
2:F:66:VAL:O	2:F:67:LYS:C	2.57	0.48
2:F:157:ARG:HE	2:J:8:THR:CG2	2.26	0.48
2:D:30:TYR:CD2	2:F:159:GLY:HA2	2.46	0.48
2:L:145:SER:O	2:L:148:LYS:HB3	2.13	0.48
1:A:75:PHE:O	1:A:76:GLU:C	2.56	0.48
2:B:37:ILE:HD12	2:B:56:LEU:HD21	1.95	0.48
2:J:68:PRO:CG	2:J:69:PHE:N	2.72	0.48
2:D:100:HIS:HA	2:H:71:ARG:HD3	1.94	0.47
2:D:151:GLU:HA	2:D:154:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:73:ILE:HG22	2:H:76:THR:HG23	1.96	0.47
1:I:31:LYS:CA	1:I:36:LYS:HB3	2.44	0.47
2:B:2:VAL:C	2:B:3:LEU:HD23	2.39	0.47
2:B:154:LYS:HD2	2:P:10:ILE:HD12	1.96	0.47
2:F:157:ARG:NE	2:J:8:THR:CG2	2.77	0.47
2:J:9:HIS:HE1	2:J:11:PHE:CE1	2.31	0.47
2:J:66:VAL:O	2:J:68:PRO:N	2.47	0.47
2:J:142:GLU:O	2:J:143:ASP:C	2.57	0.47
2:P:142:GLU:CG	2:P:143:ASP:N	2.76	0.47
1:G:60:GLN:C	1:G:62:ILE:H	2.22	0.47
2:J:37:ILE:HG23	2:J:37:ILE:O	2.14	0.47
2:J:42:ARG:HH12	2:J:52:THR:HG21	1.77	0.47
2:J:46:GLN:O	2:J:47:GLU:CG	2.63	0.47
2:L:19:SER:O	2:L:22:PHE:HB3	2.14	0.47
1:E:40:ASN:C	1:E:42:CYS:N	2.70	0.47
2:F:76:THR:HB	3:F:201:PX2:H51	1.97	0.47
2:H:113:GLN:O	2:H:121:THR:HG23	2.14	0.47
2:B:8:THR:HG22	2:H:7:SER:CB	2.34	0.47
2:D:147:THR:CG2	2:D:148:LYS:H	2.27	0.47
1:G:58:VAL:C	1:G:60:GLN:N	2.73	0.47
2:H:94:TYR:CE1	2:H:107:GLU:HG2	2.50	0.47
1:I:68:GLU:O	1:I:71:GLU:HG2	2.14	0.47
2:B:45:ASP:CB	2:B:51:ARG:NH2	2.78	0.47
2:B:57:LYS:HD2	2:B:77:TRP:CE3	2.50	0.47
1:E:38:VAL:HG23	1:E:38:VAL:O	2.15	0.47
1:G:37:SER:CA	1:G:38:VAL:HG13	2.44	0.47
1:I:54:ASN:O	1:I:58:VAL:HG23	2.13	0.47
1:I:61:GLY:O	1:I:64:PRO:HD2	2.15	0.47
1:I:66:LEU:C	1:I:68:GLU:N	2.71	0.47
2:J:3:LEU:O	2:J:4:LEU:CG	2.63	0.47
2:J:131:SER:OG	2:J:134:ASN:HB3	2.15	0.47
1:K:6:SER:CB	1:K:17:LYS:HZ1	2.28	0.47
2:L:39:THR:HG22	2:L:40:ILE:N	2.30	0.47
2:L:45:ASP:N	2:L:49:ASN:O	2.44	0.47
2:L:94:TYR:C	2:L:95:THR:HG22	2.40	0.47
2:L:157:ARG:HH11	2:L:157:ARG:HG2	1.79	0.47
1:O:32:PHE:CZ	2:P:48:GLY:O	2.68	0.47
2:P:2:VAL:CG1	2:P:128:LYS:HG3	2.44	0.47
1:A:47:TYR:O	1:A:48:ALA:C	2.58	0.47
2:F:104:MET:CB	2:F:129:PHE:HE1	2.26	0.47
2:F:147:THR:O	2:F:148:LYS:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:153:VAL:HG23	2:F:154:LYS:N	2.30	0.47
1:I:25:ASN:HB3	2:J:20:ARG:HH12	1.79	0.47
2:B:99:ASP:O	2:B:100:HIS:HB2	2.14	0.47
2:D:94:TYR:OH	2:D:96:ARG:HD3	2.15	0.47
2:D:112:TYR:OH	2:F:160:MET:HE3	2.15	0.47
2:F:58:LYS:NZ	3:F:201:PX2:H2	2.30	0.47
2:L:104:MET:O	2:L:104:MET:HG3	2.15	0.47
2:B:10:ILE:CG1	2:B:122:ILE:HG12	2.42	0.46
2:B:153:VAL:CG2	2:B:154:LYS:H	2.28	0.46
2:H:18:VAL:HA	2:P:164:ILE:HD11	1.97	0.46
1:I:31:LYS:CD	1:I:36:LYS:HG2	2.36	0.46
2:J:99:ASP:OD1	2:J:99:ASP:N	2.48	0.46
2:N:4:LEU:H	2:N:4:LEU:HG	1.43	0.46
2:N:150:ASP:O	2:N:154:LYS:HG3	2.14	0.46
2:F:62:LEU:H	2:F:62:LEU:CD1	2.23	0.46
2:H:146:ARG:HA	2:P:5:HIS:CE1	2.50	0.46
2:J:157:ARG:C	2:J:159:GLY:N	2.72	0.46
1:K:62:ILE:HG23	1:K:62:ILE:O	2.14	0.46
2:L:113:GLN:O	2:L:121:THR:HA	2.15	0.46
2:B:85:ASN:HB3	2:B:88:ASN:OD1	2.15	0.46
2:B:106:VAL:HB	3:B:201:PX2:H12	1.97	0.46
2:D:88:ASN:OD1	2:D:90:THR:HB	2.16	0.46
2:L:94:TYR:C	2:L:95:THR:CG2	2.89	0.46
2:D:51:ARG:HD3	2:D:83:VAL:HG22	1.97	0.46
2:D:59:SER:O	2:D:60:GLY:C	2.57	0.46
2:D:154:LYS:O	2:D:158:MET:HG3	2.15	0.46
1:E:43:SER:O	1:E:46:TRP:HB3	2.15	0.46
1:I:36:LYS:HD3	1:I:37:SER:H	1.81	0.46
1:G:40:ASN:CG	1:G:41:GLU:N	2.72	0.46
2:J:65:TRP:CD1	2:J:66:VAL:HG23	2.51	0.46
2:J:66:VAL:N	2:J:68:PRO:HD2	2.30	0.46
2:L:3:LEU:O	2:L:5:HIS:CE1	2.68	0.46
2:L:73:ILE:HG22	2:L:74:THR:H	1.80	0.46
2:B:97:ASN:HB3	3:B:201:PX2:C9	2.34	0.46
2:F:3:LEU:C	2:F:4:LEU:HD12	2.40	0.46
1:I:69:ALA:C	1:I:71:GLU:N	2.73	0.46
1:K:63:LYS:H	1:K:64:PRO:HD2	1.79	0.46
2:L:44:VAL:HG12	2:L:45:ASP:O	2.16	0.46
2:P:131:SER:O	2:P:131:SER:OG	2.31	0.46
2:B:103:ILE:HG21	3:B:201:PX2:H29	1.97	0.46
2:D:80:GLU:HA	2:D:95:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:ILE:O	1:G:5:MET:HE2	2.16	0.46
2:H:69:PHE:HB2	2:H:71:ARG:HD2	1.97	0.46
2:D:5:HIS:HD2	2:F:150:ASP:OD1	1.99	0.46
2:D:63:PRO:HB2	2:D:68:PRO:CG	2.46	0.46
2:J:68:PRO:C	2:J:70:LEU:N	2.73	0.46
1:K:42:CYS:C	1:K:44:LYS:N	2.74	0.46
2:L:125:SER:O	2:L:126:ARG:HG3	2.15	0.46
2:B:88:ASN:O	2:B:90:THR:HG23	2.16	0.46
2:B:136:GLY:O	2:B:137:ILE:C	2.57	0.46
2:D:69:PHE:CD1	2:D:69:PHE:C	2.94	0.46
2:F:96:ARG:HG3	2:F:97:ASN:O	2.16	0.46
2:H:5:HIS:HD2	2:P:146:ARG:HA	1.81	0.46
2:H:28:ASN:OD1	2:H:30:TYR:N	2.42	0.46
1:K:42:CYS:O	1:K:44:LYS:N	2.49	0.46
2:L:13:THR:HG22	2:L:14:ASP:N	2.30	0.46
1:M:54:ASN:O	1:M:58:VAL:HG23	2.16	0.46
2:B:37:ILE:HD11	2:B:54:ARG:CZ	2.46	0.46
2:B:114:PHE:CE2	2:B:116:SER:HA	2.51	0.46
2:B:157:ARG:O	2:B:158:MET:C	2.59	0.46
2:F:110:THR:HG22	2:F:111:THR:N	2.31	0.46
2:P:13:THR:HG22	2:P:14:ASP:N	2.31	0.46
1:A:62:ILE:HG13	1:A:62:ILE:O	2.15	0.45
2:D:7:SER:HA	2:J:6:LYS:O	2.15	0.45
2:D:32:PRO:C	2:D:34:VAL:H	2.25	0.45
1:E:9:PHE:CD1	1:E:9:PHE:C	2.94	0.45
2:F:49:ASN:OD1	2:F:85:ASN:ND2	2.35	0.45
2:N:162:PHE:O	2:N:163:VAL:C	2.59	0.45
1:A:13:CYS:O	1:A:14:THR:C	2.57	0.45
2:F:31:SER:N	2:F:32:PRO:CD	2.79	0.45
1:A:15:ASP:C	1:A:17:LYS:N	2.73	0.45
2:J:3:LEU:CB	2:J:129:PHE:HD2	2.28	0.45
2:J:15:PHE:CD1	2:J:15:PHE:C	2.93	0.45
2:L:42:ARG:HH21	2:L:42:ARG:CG	2.30	0.45
2:P:39:THR:HA	2:P:54:ARG:HG2	1.98	0.45
1:C:31:LYS:HB3	1:C:36:LYS:O	2.16	0.45
2:H:111:THR:O	2:H:111:THR:CG2	2.64	0.45
2:B:96:ARG:CB	2:B:106:VAL:O	2.65	0.45
2:B:100:HIS:C	2:B:102:GLY:N	2.74	0.45
1:C:8:SER:HA	2:D:38:ASP:OD1	2.16	0.45
2:D:11:PHE:C	2:D:13:THR:H	2.24	0.45
2:D:35:LEU:HD12	2:D:57:LYS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:PHE:C	2:D:69:PHE:HD1	2.24	0.45
1:E:50:THR:CG2	1:E:51:THR:N	2.79	0.45
2:F:159:GLY:O	2:F:162:PHE:HB3	2.17	0.45
2:J:164:ILE:HG13	2:L:21:ALA:CB	2.46	0.45
1:C:74:PRO:HB3	2:D:94:TYR:CE1	2.52	0.45
2:D:63:PRO:O	2:D:65:TRP:N	2.50	0.45
2:D:157:ARG:NH2	2:F:7:SER:OG	2.49	0.45
1:E:39:GLU:N	1:E:39:GLU:CD	2.75	0.45
1:K:47:TYR:CD1	1:K:47:TYR:C	2.94	0.45
2:L:22:PHE:O	2:L:25:ARG:CG	2.58	0.45
2:L:146:ARG:C	2:L:148:LYS:N	2.74	0.45
2:P:42:ARG:NH2	2:P:52:THR:HG21	2.32	0.45
2:D:45:ASP:OD1	2:D:49:ASN:HB2	2.17	0.45
2:D:106:VAL:HG11	2:F:149:PHE:CZ	2.51	0.45
2:F:88:ASN:OD1	2:F:88:ASN:N	2.50	0.45
2:F:140:LYS:HG2	2:F:141:VAL:N	2.32	0.45
2:L:85:ASN:ND2	2:L:88:ASN:OD1	2.49	0.45
2:D:6:LYS:O	2:D:6:LYS:HG2	2.17	0.45
1:E:42:CYS:HA	1:E:45:GLN:OE1	2.17	0.45
2:F:45:ASP:OD1	2:F:47:GLU:HB2	2.17	0.45
2:N:4:LEU:O	2:N:5:HIS:CG	2.69	0.45
1:O:24:PHE:CZ	2:P:50:LEU:HD21	2.52	0.45
1:E:39:GLU:CD	1:E:39:GLU:H	2.23	0.45
2:H:29:PRO:HD2	2:P:162:PHE:CD2	2.52	0.45
1:I:73:ALA:O	1:I:76:GLU:N	2.45	0.45
2:N:134:ASN:OD1	2:N:135:MET:N	2.50	0.45
2:B:29:PRO:HG2	2:N:162:PHE:CD2	2.52	0.45
2:B:115:ASP:O	2:B:116:SER:C	2.60	0.45
2:B:146:ARG:O	2:B:150:ASP:HB2	2.16	0.45
2:F:3:LEU:O	2:F:4:LEU:CG	2.61	0.45
1:G:66:LEU:HD22	2:H:55:LEU:HD22	1.99	0.45
2:H:69:PHE:CD2	2:H:70:LEU:N	2.85	0.45
1:I:29:SER:OG	2:J:20:ARG:HD2	2.17	0.45
2:F:111:THR:HG22	2:F:124:ASP:HB3	1.99	0.44
1:I:9:PHE:CD1	1:I:9:PHE:C	2.94	0.44
2:J:111:THR:O	2:J:111:THR:CG2	2.64	0.44
2:L:110:THR:HG22	2:L:111:THR:N	2.32	0.44
1:M:27:TRP:O	1:M:31:LYS:HB2	2.17	0.44
2:N:137:ILE:C	2:N:139:SER:N	2.73	0.44
2:D:50:LEU:HA	2:D:50:LEU:HD12	1.76	0.44
1:E:10:ALA:HB1	1:E:12:GLU:CD	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:CYS:O	1:E:43:SER:C	2.59	0.44
2:H:9:HIS:CD2	2:P:157:ARG:HD3	2.52	0.44
2:H:91:MET:HB3	2:H:112:TYR:HB2	1.99	0.44
1:I:36:LYS:NZ	1:I:36:LYS:CB	2.81	0.44
2:N:153:VAL:O	2:N:157:ARG:HG2	2.16	0.44
1:A:17:LYS:HB2	1:A:49:TYR:CE1	2.52	0.44
1:E:50:THR:HG22	1:E:51:THR:N	2.32	0.44
2:F:158:MET:O	2:F:159:GLY:C	2.58	0.44
2:L:94:TYR:CD1	2:L:95:THR:N	2.85	0.44
2:D:70:LEU:CD1	2:D:70:LEU:N	2.79	0.44
1:E:39:GLU:HG2	1:E:41:GLU:OE2	2.17	0.44
2:F:79:ILE:HG21	2:F:98:LEU:HD23	1.99	0.44
2:J:65:TRP:C	2:J:68:PRO:HD2	2.42	0.44
2:J:69:PHE:O	2:J:71:ARG:N	2.51	0.44
2:L:142:GLU:C	2:L:144:TRP:N	2.73	0.44
1:M:17:LYS:HB2	1:M:49:TYR:CE1	2.52	0.44
2:F:10:ILE:HG23	2:F:122:ILE:CD1	2.48	0.44
2:F:98:LEU:HD13	2:F:98:LEU:O	2.18	0.44
2:N:137:ILE:O	2:N:139:SER:N	2.50	0.44
1:O:17:LYS:HB2	1:O:49:TYR:CE1	2.52	0.44
2:B:118:THR:C	2:B:120:SER:N	2.75	0.44
2:D:22:PHE:HA	2:F:160:MET:HE1	2.00	0.44
2:F:67:LYS:CB	2:F:68:PRO:CD	2.95	0.44
2:H:50:LEU:O	2:H:83:VAL:HA	2.18	0.44
2:H:118:THR:O	2:H:119:SER:HB2	2.17	0.44
1:I:6:SER:HB3	1:I:17:LYS:HZ1	1.83	0.44
2:J:45:ASP:OD1	2:J:49:ASN:HB2	2.18	0.44
2:J:68:PRO:O	2:J:70:LEU:N	2.50	0.44
2:J:133:PHE:O	2:J:134:ASN:C	2.59	0.44
2:B:141:VAL:O	2:B:144:TRP:HB3	2.18	0.44
2:D:29:PRO:HG3	2:F:162:PHE:CE2	2.53	0.44
2:D:115:ASP:O	2:D:116:SER:C	2.60	0.44
2:F:44:VAL:HG12	2:F:48:GLY:HA2	1.98	0.44
1:I:6:SER:CB	1:I:17:LYS:HZ1	2.31	0.44
2:J:42:ARG:NH1	2:J:52:THR:CG2	2.81	0.44
2:L:56:LEU:N	2:L:56:LEU:HD12	2.33	0.44
1:O:73:ALA:HA	1:O:74:PRO:HD3	1.73	0.44
3:F:201:PX2:H17	3:F:201:PX2:H12	1.76	0.44
1:K:42:CYS:C	1:K:44:LYS:H	2.25	0.44
1:K:51:THR:C	1:K:53:VAL:N	2.75	0.44
2:L:44:VAL:HG13	2:L:49:ASN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LEU:O	2:B:71:ARG:O	2.35	0.44
2:B:137:ILE:O	2:B:140:LYS:HB2	2.18	0.44
1:C:11:PRO:C	1:C:13:CYS:N	2.76	0.44
2:H:66:VAL:O	2:H:66:VAL:HG23	2.18	0.44
2:L:40:ILE:HG22	2:L:41:SER:N	2.33	0.44
2:L:42:ARG:O	2:L:43:ASN:CB	2.66	0.44
2:H:42:ARG:HH21	2:H:52:THR:HG21	1.81	0.43
1:K:32:PHE:CE2	2:L:86:PRO:HG2	2.53	0.43
2:P:50:LEU:HB3	2:P:84:VAL:HB	2.00	0.43
2:B:25:ARG:NH2	2:B:26:TYR:CE2	2.86	0.43
2:B:64:THR:C	2:B:66:VAL:H	2.24	0.43
2:B:155:LYS:HA	2:B:158:MET:CE	2.48	0.43
2:D:102:GLY:H	2:H:71:ARG:HH21	1.66	0.43
2:D:107:GLU:HB2	2:D:128:LYS:HG3	2.00	0.43
3:F:201:PX2:H7	3:F:201:PX2:H30	1.99	0.43
1:K:17:LYS:O	1:K:19:LYS:N	2.51	0.43
2:L:46:GLN:HE21	2:L:46:GLN:HB3	1.57	0.43
2:P:169:GLU:H	2:P:169:GLU:HG3	1.57	0.43
2:B:0:PRO:CB	2:B:131:SER:OG	2.67	0.43
2:B:57:LYS:HD2	2:B:77:TRP:CE2	2.52	0.43
2:D:63:PRO:CB	2:D:68:PRO:HD3	2.47	0.43
2:H:25:ARG:NH1	2:H:80:GLU:OE1	2.50	0.43
1:I:41:GLU:C	1:I:43:SER:H	2.26	0.43
2:J:145:SER:O	2:J:148:LYS:N	2.49	0.43
2:J:149:PHE:CE1	2:L:5:HIS:O	2.71	0.43
1:K:59:LYS:NZ	1:K:59:LYS:HB3	2.33	0.43
2:D:153:VAL:O	2:D:154:LYS:C	2.60	0.43
1:I:6:SER:OG	2:J:26:TYR:O	2.36	0.43
1:K:12:GLU:HG3	1:K:52:CYS:SG	2.58	0.43
2:L:50:LEU:CD1	2:L:51:ARG:O	2.66	0.43
2:L:126:ARG:HB2	2:L:126:ARG:NH1	2.34	0.43
2:D:22:PHE:CD2	2:D:91:MET:HE1	2.54	0.43
2:H:57:LYS:HG3	2:H:77:TRP:CZ2	2.53	0.43
1:I:66:LEU:HD21	2:J:40:ILE:HG21	2.01	0.43
2:L:50:LEU:HD12	2:L:51:ARG:N	2.33	0.43
2:L:73:ILE:H	2:L:73:ILE:CD1	2.03	0.43
2:B:137:ILE:C	2:B:141:VAL:CG1	2.92	0.43
1:C:47:TYR:HA	1:C:50:THR:HG22	2.01	0.43
2:F:28:ASN:C	2:F:28:ASN:OD1	2.62	0.43
2:J:70:LEU:C	2:J:72:GLY:N	2.72	0.43
2:J:99:ASP:O	2:J:100:HIS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:84:VAL:C	2:L:86:PRO:HD3	2.43	0.43
1:K:28:TYR:OH	1:K:33:LEU:HD21	2.17	0.43
2:N:3:LEU:O	2:N:128:LYS:HA	2.19	0.43
2:P:129:PHE:N	2:P:129:PHE:HD1	2.17	0.43
1:A:61:GLY:O	1:A:64:PRO:HD2	2.19	0.43
2:B:96:ARG:HB3	2:B:107:GLU:HA	1.99	0.43
2:B:157:ARG:HG2	2:B:157:ARG:NH1	2.32	0.43
2:D:42:ARG:HE	2:D:52:THR:CG2	2.32	0.43
2:J:22:PHE:CD1	2:J:22:PHE:C	2.96	0.43
2:L:45:ASP:OD2	2:L:49:ASN:ND2	2.52	0.43
2:N:3:LEU:HD22	2:N:3:LEU:O	2.17	0.43
1:A:40:ASN:O	1:A:42:CYS:N	2.52	0.43
1:C:57:LEU:HA	1:C:62:ILE:HG22	2.01	0.43
2:F:101:THR:HA	2:F:104:MET:O	2.19	0.43
2:F:166:LYS:HG3	2:F:167:LEU:N	2.33	0.43
2:H:58:LYS:HE3	2:H:78:ILE:HD12	2.00	0.43
1:I:31:LYS:CB	1:I:36:LYS:HB3	2.46	0.43
2:L:47:GLU:OE1	2:L:47:GLU:N	2.50	0.43
2:L:105:LYS:HB3	2:L:130:SER:HB2	2.01	0.43
2:P:165:GLN:C	2:P:167:LEU:N	2.75	0.43
2:B:90:THR:HA	2:B:112:TYR:O	2.19	0.43
1:C:11:PRO:C	1:C:13:CYS:H	2.25	0.43
1:E:47:TYR:C	1:E:47:TYR:CD1	2.97	0.43
1:I:36:LYS:HA	1:I:36:LYS:NZ	2.33	0.43
1:I:38:VAL:HG22	1:I:39:GLU:N	2.34	0.43
2:J:85:ASN:HB3	2:J:90:THR:HG22	2.00	0.43
2:L:160:MET:O	2:L:161:ALA:C	2.61	0.43
2:P:3:LEU:O	2:P:4:LEU:CB	2.63	0.43
1:A:60:GLN:HB3	1:A:62:ILE:HG22	2.01	0.42
2:D:67:LYS:N	2:D:68:PRO:HD2	2.29	0.42
1:G:50:THR:HG23	1:G:51:THR:N	2.34	0.42
2:B:57:LYS:HB2	2:B:77:TRP:CZ3	2.55	0.42
2:D:42:ARG:HB2	2:D:52:THR:HG23	2.01	0.42
2:F:122:ILE:HG12	2:J:158:MET:CG	2.48	0.42
1:G:32:PHE:CZ	2:H:86:PRO:HD3	2.54	0.42
1:E:30:GLU:O	1:E:34:LYS:HB2	2.18	0.42
2:F:68:PRO:C	2:F:70:LEU:N	2.77	0.42
1:K:17:LYS:C	1:K:19:LYS:N	2.74	0.42
2:L:37:ILE:HA	2:L:55:LEU:O	2.19	0.42
2:N:26:TYR:CE2	2:N:56:LEU:HD21	2.54	0.42
1:A:24:PHE:O	1:A:28:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45:ASP:C	2:F:47:GLU:N	2.76	0.42
2:F:105:LYS:HB3	2:F:130:SER:HB2	2.01	0.42
2:F:162:PHE:O	2:F:163:VAL:C	2.60	0.42
2:H:8:THR:HG22	2:N:157:ARG:HH21	1.84	0.42
1:I:25:ASN:HB3	2:J:20:ARG:CZ	2.49	0.42
1:I:36:LYS:HB2	1:I:36:LYS:NZ	2.34	0.42
2:J:85:ASN:OD1	2:J:87:ALA:HB3	2.19	0.42
2:J:159:GLY:HA2	2:L:30:TYR:CD2	2.54	0.42
1:K:47:TYR:CD1	1:K:47:TYR:O	2.72	0.42
2:L:142:GLU:O	2:L:143:ASP:C	2.63	0.42
2:N:168:GLU:C	2:N:169:GLU:HG3	2.44	0.42
1:C:20:TYR:OH	2:D:42:ARG:HD2	2.19	0.42
2:H:25:ARG:NH2	2:H:26:TYR:HE2	2.18	0.42
2:J:4:LEU:HB3	2:J:5:HIS:H	1.36	0.42
2:L:15:PHE:CG	2:L:89:SER:HB3	2.55	0.42
2:P:4:LEU:O	2:P:5:HIS:HB3	2.19	0.42
2:B:64:THR:O	2:B:68:PRO:HD3	2.20	0.42
2:B:118:THR:C	2:B:120:SER:H	2.28	0.42
2:D:63:PRO:HB2	2:D:68:PRO:HG3	2.02	0.42
2:H:62:LEU:O	2:H:64:THR:N	2.53	0.42
2:N:11:PHE:C	2:N:13:THR:H	2.27	0.42
1:O:62:ILE:HG13	1:O:62:ILE:O	2.20	0.42
2:P:131:SER:C	2:P:133:PHE:N	2.78	0.42
2:B:76:THR:HG22	2:B:77:TRP:N	2.34	0.42
2:F:11:PHE:O	2:F:120:SER:HB2	2.19	0.42
2:L:104:MET:HA	2:L:130:SER:O	2.20	0.42
2:P:154:LYS:HB2	2:P:154:LYS:NZ	2.34	0.42
2:F:45:ASP:C	2:F:47:GLU:H	2.28	0.42
2:F:153:VAL:O	2:F:157:ARG:HG3	2.20	0.42
1:K:5:MET:HA	1:K:5:MET:CE	2.45	0.42
1:K:57:LEU:HB3	1:K:63:LYS:HE2	2.00	0.42
2:L:165:GLN:O	2:L:169:GLU:HG3	2.20	0.42
2:B:62:LEU:HA	2:B:63:PRO:HD3	1.91	0.42
2:F:6:LYS:HE3	2:F:126:ARG:HG2	2.02	0.42
1:G:68:GLU:C	1:G:70:ARG:H	2.28	0.42
1:I:10:ALA:O	1:I:12:GLU:N	2.52	0.42
2:L:145:SER:HA	2:L:148:LYS:HB3	2.01	0.42
2:N:94:TYR:HA	2:N:108:GLU:O	2.19	0.42
2:D:42:ARG:NE	2:D:52:THR:CG2	2.83	0.42
1:E:44:LYS:HE3	1:E:44:LYS:HB2	1.95	0.42
1:E:46:TRP:O	1:E:49:TYR:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:58:LYS:CG	2:F:78:ILE:HD12	2.48	0.42
2:H:2:VAL:O	2:H:3:LEU:HD23	2.20	0.42
2:H:73:ILE:HD12	2:H:73:ILE:C	2.45	0.42
2:H:88:ASN:OD1	2:H:90:THR:CB	2.68	0.42
2:J:35:LEU:HB2	2:J:57:LYS:HD2	2.02	0.42
2:J:153:VAL:O	2:J:157:ARG:HG3	2.19	0.42
2:L:69:PHE:CG	2:L:70:LEU:N	2.86	0.42
2:P:94:TYR:HA	2:P:108:GLU:O	2.19	0.42
2:D:4:LEU:HB3	2:D:5:HIS:H	1.39	0.41
2:D:37:ILE:HA	2:D:55:LEU:O	2.20	0.41
2:D:69:PHE:HD1	2:D:69:PHE:O	2.02	0.41
2:F:57:LYS:HE2	2:F:75:GLU:OE2	2.19	0.41
2:F:80:GLU:CB	2:F:95:THR:HG22	2.49	0.41
1:I:31:LYS:CA	1:I:36:LYS:CB	2.97	0.41
2:J:162:PHE:CE2	2:L:29:PRO:HD3	2.55	0.41
1:M:6:SER:CB	2:N:27:PRO:HD3	2.50	0.41
2:N:166:LYS:HG3	2:N:167:LEU:H	1.84	0.41
1:C:25:ASN:HB3	2:D:20:ARG:CZ	2.50	0.41
2:D:102:GLY:N	2:H:71:ARG:NH2	2.68	0.41
2:F:88:ASN:O	2:F:89:SER:C	2.62	0.41
1:G:37:SER:C	1:G:38:VAL:HG13	2.45	0.41
2:J:62:LEU:C	2:J:64:THR:N	2.77	0.41
1:K:16:LEU:CD1	1:K:52:CYS:HB2	2.50	0.41
2:N:79:ILE:O	2:N:95:THR:HA	2.20	0.41
2:D:37:ILE:HD11	2:D:54:ARG:CZ	2.50	0.41
2:D:67:LYS:N	2:D:68:PRO:HD3	2.31	0.41
1:E:47:TYR:O	1:E:48:ALA:C	2.63	0.41
2:F:136:GLY:O	2:F:137:ILE:C	2.62	0.41
2:H:26:TYR:HE1	2:H:31:SER:CB	2.32	0.41
2:H:59:SER:HA	2:H:75:GLU:CB	2.50	0.41
1:I:30:GLU:OE1	1:I:30:GLU:HA	2.19	0.41
1:I:73:ALA:O	1:I:75:PHE:N	2.52	0.41
2:P:165:GLN:O	2:P:166:LYS:C	2.63	0.41
1:A:47:TYR:CA	1:A:50:THR:HG22	2.50	0.41
2:B:147:THR:HA	2:B:150:ASP:HB3	2.01	0.41
2:B:148:LYS:HD3	2:B:148:LYS:C	2.44	0.41
2:B:154:LYS:O	2:B:158:MET:HG3	2.21	0.41
2:D:44:VAL:HA	2:D:49:ASN:O	2.21	0.41
1:G:68:GLU:C	1:G:70:ARG:N	2.78	0.41
2:L:114:PHE:CD1	2:L:114:PHE:C	2.98	0.41
2:L:131:SER:C	2:L:133:PHE:N	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:56:LEU:N	2:J:78:ILE:O	2.53	0.41
2:J:154:LYS:CG	2:J:158:MET:HE2	2.48	0.41
1:K:45:GLN:N	1:K:45:GLN:OE1	2.53	0.41
2:L:110:THR:HA	2:L:125:SER:HA	2.03	0.41
2:P:2:VAL:HG13	2:P:128:LYS:HG2	2.02	0.41
2:P:8:THR:HG22	2:P:9:HIS:N	2.35	0.41
1:C:58:VAL:HG22	1:C:63:LYS:HD3	2.02	0.41
2:D:30:TYR:HD2	2:F:159:GLY:CA	2.31	0.41
2:J:26:TYR:HE2	2:J:56:LEU:HD21	1.86	0.41
2:J:160:MET:HE1	2:L:112:TYR:CZ	2.55	0.41
1:O:39:GLU:H	1:O:39:GLU:HG2	1.75	0.41
2:P:133:PHE:HD1	2:P:134:ASN:N	2.17	0.41
2:B:42:ARG:O	2:B:43:ASN:HB3	2.20	0.41
2:D:62:LEU:O	2:D:63:PRO:C	2.64	0.41
2:J:103:ILE:O	2:J:104:MET:HG3	2.21	0.41
1:K:10:ALA:CB	1:K:12:GLU:HG2	2.50	0.41
2:L:73:ILE:HD12	2:L:100:HIS:NE2	2.35	0.41
2:L:129:PHE:CD1	2:L:130:SER:N	2.88	0.41
1:C:21:ASP:O	1:C:22:SER:C	2.63	0.41
1:C:50:THR:HG23	1:C:51:THR:N	2.34	0.41
2:D:140:LYS:O	2:D:141:VAL:C	2.62	0.41
2:J:91:MET:HB3	2:J:112:TYR:HB2	2.03	0.41
2:L:14:ASP:O	2:L:15:PHE:C	2.63	0.41
2:P:133:PHE:C	2:P:135:MET:N	2.77	0.41
2:B:22:PHE:CD2	2:B:91:MET:HE1	2.56	0.41
2:B:64:THR:O	2:B:66:VAL:N	2.54	0.41
2:B:66:VAL:C	2:B:68:PRO:HD2	2.45	0.41
2:B:110:THR:HG23	2:B:125:SER:OG	2.21	0.41
1:E:41:GLU:CD	1:E:41:GLU:H	2.26	0.41
2:F:14:ASP:OD1	2:F:17:SER:N	2.45	0.41
2:F:157:ARG:CD	2:J:8:THR:CG2	2.99	0.41
1:G:24:PHE:O	1:G:25:ASN:C	2.63	0.41
2:H:140:LYS:HG2	2:H:141:VAL:N	2.34	0.41
1:I:53:VAL:O	1:I:54:ASN:C	2.64	0.41
2:J:157:ARG:O	2:J:158:MET:C	2.63	0.41
1:K:16:LEU:HD13	1:K:52:CYS:HB2	2.01	0.41
1:K:70:ARG:CZ	2:L:40:ILE:CG2	2.99	0.41
2:N:96:ARG:HA	2:N:106:VAL:O	2.20	0.41
2:N:135:MET:HE3	2:N:135:MET:HB3	1.72	0.41
1:O:24:PHE:HZ	2:P:50:LEU:HD21	1.85	0.41
1:O:32:PHE:HZ	2:P:48:GLY:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:160:MET:O	2:P:164:ILE:HG12	2.20	0.41
2:D:10:ILE:HD12	2:D:10:ILE:N	2.32	0.41
2:D:42:ARG:NH2	2:D:52:THR:HG21	2.35	0.41
2:F:7:SER:HB2	2:L:8:THR:O	2.21	0.41
2:F:22:PHE:CE1	2:F:25:ARG:NH1	2.81	0.41
1:G:54:ASN:HA	1:G:57:LEU:HD12	2.02	0.41
2:H:5:HIS:HB2	2:H:127:VAL:HB	2.03	0.41
1:I:31:LYS:HA	1:I:36:LYS:CB	2.51	0.41
2:P:111:THR:O	2:P:123:ALA:HA	2.21	0.41
1:A:7:ALA:O	2:B:36:SER:HB2	2.21	0.40
2:B:143:ASP:HA	2:B:146:ARG:HD2	2.01	0.40
2:D:13:THR:HG22	2:D:14:ASP:N	2.36	0.40
2:H:33:HIS:HD2	2:H:58:LYS:HD3	1.85	0.40
2:H:67:LYS:N	2:H:68:PRO:HD2	2.35	0.40
2:H:115:ASP:HB2	2:N:158:MET:HE1	2.03	0.40
2:J:107:GLU:HB2	2:J:128:LYS:HD3	2.03	0.40
1:K:49:TYR:HH	2:L:38:ASP:CG	2.29	0.40
2:N:8:THR:CG2	2:P:9:HIS:HD2	2.34	0.40
2:P:131:SER:C	2:P:133:PHE:H	2.28	0.40
2:P:133:PHE:C	2:P:135:MET:H	2.29	0.40
2:B:66:VAL:HG12	2:B:66:VAL:O	2.21	0.40
2:D:13:THR:HG21	2:D:17:SER:HB3	2.01	0.40
2:D:51:ARG:HH21	2:D:51:ARG:CG	2.34	0.40
2:F:115:ASP:OD2	2:L:30:TYR:OH	2.38	0.40
1:G:6:SER:CB	1:G:17:LYS:HZ3	2.29	0.40
1:G:38:VAL:N	1:G:39:GLU:OE1	2.43	0.40
2:J:107:GLU:HB2	2:J:128:LYS:CD	2.51	0.40
2:L:50:LEU:HD12	2:L:50:LEU:C	2.46	0.40
2:N:73:ILE:CG1	2:N:74:THR:H	2.32	0.40
1:E:60:GLN:C	1:E:62:ILE:N	2.77	0.40
2:F:157:ARG:HH11	2:F:157:ARG:CG	2.30	0.40
2:H:1:MET:HG2	2:H:2:VAL:N	2.36	0.40
2:H:2:VAL:O	2:H:3:LEU:CD2	2.69	0.40
1:I:69:ALA:O	1:I:71:GLU:N	2.54	0.40
1:C:27:TRP:CH2	1:C:32:PHE:HB2	2.56	0.40
1:C:57:LEU:HA	1:C:62:ILE:CG2	2.51	0.40
2:D:42:ARG:HH21	2:D:52:THR:HG21	1.86	0.40
2:F:141:VAL:C	2:F:143:ASP:N	2.78	0.40
1:I:19:LYS:O	1:I:20:TYR:C	2.62	0.40
1:K:58:VAL:C	1:K:60:GLN:H	2.29	0.40
1:A:9:PHE:CD1	1:A:9:PHE:C	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:ASP:O	2:B:146:ARG:HB2	2.22	0.40
2:D:62:LEU:HD23	2:D:62:LEU:N	2.37	0.40
2:F:25:ARG:HD2	2:F:26:TYR:OH	2.21	0.40
2:F:25:ARG:HH22	2:F:56:LEU:HD21	1.86	0.40
2:F:96:ARG:HA	2:F:106:VAL:O	2.21	0.40
2:H:76:THR:HG22	2:H:77:TRP:N	2.37	0.40
2:H:141:VAL:O	2:H:144:TRP:HB3	2.21	0.40
2:J:145:SER:O	2:J:146:ARG:C	2.65	0.40
2:L:96:ARG:NH2	2:L:96:ARG:HG3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	71/81 (88%)	54 (76%)	10 (14%)	7 (10%)	0	2
1	C	71/81 (88%)	54 (76%)	15 (21%)	2 (3%)	4	25
1	E	71/81 (88%)	52 (73%)	16 (22%)	3 (4%)	2	16
1	G	71/81 (88%)	54 (76%)	15 (21%)	2 (3%)	4	25
1	I	71/81 (88%)	52 (73%)	8 (11%)	11 (16%)	0	0
1	K	71/81 (88%)	50 (70%)	17 (24%)	4 (6%)	1	11
1	M	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
1	O	66/81 (82%)	63 (96%)	3 (4%)	0	100	100
2	B	158/184 (86%)	133 (84%)	19 (12%)	6 (4%)	2	18
2	D	168/184 (91%)	137 (82%)	20 (12%)	11 (6%)	1	8
2	F	165/184 (90%)	129 (78%)	28 (17%)	8 (5%)	2	14
2	H	160/184 (87%)	130 (81%)	25 (16%)	5 (3%)	3	22
2	J	167/184 (91%)	130 (78%)	27 (16%)	10 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	167/184 (91%)	128 (77%)	27 (16%)	12 (7%)	1	6
2	N	153/184 (83%)	139 (91%)	11 (7%)	3 (2%)	6	31
2	P	155/184 (84%)	144 (93%)	8 (5%)	3 (2%)	6	33
All	All	1856/2120 (88%)	1518 (82%)	251 (14%)	87 (5%)	2	14

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	71	ARG
1	C	40	ASN
2	D	5	HIS
2	D	63	PRO
2	D	64	THR
2	D	65	TRP
2	D	67	LYS
2	D	68	PRO
1	E	37	SER
2	F	131	SER
2	H	70	LEU
2	H	87	ALA
1	I	38	VAL
2	J	2	VAL
2	J	5	HIS
2	J	37	ILE
2	L	2	VAL
2	L	63	PRO
2	L	68	PRO
2	L	69	PHE
2	P	132	GLY
1	A	40	ASN
1	A	41	GLU
2	B	65	TRP
2	B	66	VAL
2	D	117	ALA
1	E	40	ASN
1	G	44	LYS
1	I	31	LYS
1	I	42	CYS
1	I	67	ASP
2	J	47	GLU
2	J	63	PRO

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Mol	Chain	Res	Type
2	J	131	SER
2	J	152	ASN
2	L	64	THR
2	L	70	LEU
2	N	4	LEU
2	N	5	HIS
2	N	74	THR
2	P	133	PHE
1	A	39	GLU
1	A	44	LYS
2	B	29	PRO
2	D	46	GLN
2	D	141	VAL
2	F	4	LEU
2	F	5	HIS
2	F	101	THR
2	H	72	GLY
1	I	11	PRO
1	I	66	LEU
1	I	70	ARG
1	K	11	PRO
1	K	43	SER
2	L	4	LEU
2	L	28	ASN
2	L	43	ASN
2	P	4	LEU
1	A	37	SER
1	A	48	ALA
2	B	134	ASN
1	C	26	GLU
2	D	33	HIS
2	F	69	PHE
2	F	100	HIS
2	H	69	PHE
1	I	27	TRP
1	I	32	PHE
2	J	104	MET
2	J	133	PHE
1	K	30	GLU
2	L	13	THR
2	J	150	ASP
2	L	117	ALA

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Mol	Chain	Res	Type
2	B	31	SER
1	E	46	TRP
2	H	41	SER
1	I	49	TYR
2	D	66	VAL
1	G	61	GLY
1	K	38	VAL
2	F	37	ILE
2	L	67	LYS
1	A	38	VAL
1	I	74	PRO
2	F	73	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	63/68 (93%)	59 (94%)	4 (6%)	16	48
1	C	62/68 (91%)	58 (94%)	4 (6%)	15	47
1	E	63/68 (93%)	56 (89%)	7 (11%)	6	25
1	G	63/68 (93%)	56 (89%)	7 (11%)	6	25
1	I	63/68 (93%)	53 (84%)	10 (16%)	2	13
1	K	63/68 (93%)	60 (95%)	3 (5%)	23	56
1	M	63/68 (93%)	61 (97%)	2 (3%)	34	65
1	O	59/68 (87%)	56 (95%)	3 (5%)	21	54
2	B	145/169 (86%)	130 (90%)	15 (10%)	7	28
2	D	150/169 (89%)	132 (88%)	18 (12%)	5	23
2	F	148/169 (88%)	136 (92%)	12 (8%)	11	39
2	H	133/169 (79%)	111 (84%)	22 (16%)	2	12
2	J	148/169 (88%)	123 (83%)	25 (17%)	2	11
2	L	148/169 (88%)	120 (81%)	28 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	143/169 (85%)	132 (92%)	11 (8%)	12	41
2	P	142/169 (84%)	136 (96%)	6 (4%)	26	60
All	All	1656/1896 (87%)	1479 (89%)	177 (11%)	6	27

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	CYS
1	A	38	VAL
1	A	40	ASN
1	A	66	LEU
2	B	8	THR
2	B	13	THR
2	B	30	TYR
2	B	37	ILE
2	B	49	ASN
2	B	64	THR
2	B	80	GLU
2	B	95	THR
2	B	101	THR
2	B	111	THR
2	B	113	GLN
2	B	130	SER
2	B	137	ILE
2	B	141	VAL
2	B	154	LYS
1	C	18	THR
1	C	38	VAL
1	C	43	SER
1	C	68	GLU
2	D	10	ILE
2	D	25	ARG
2	D	33	HIS
2	D	52	THR
2	D	59	SER
2	D	62	LEU
2	D	63	PRO
2	D	68	PRO
2	D	69	PHE
2	D	70	LEU
2	D	74	THR

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Mol	Chain	Res	Type
2	D	90	THR
2	D	94	TYR
2	D	98	LEU
2	D	125	SER
2	D	135	MET
2	D	149	PHE
2	D	157	ARG
1	E	39	GLU
1	E	41	GLU
1	E	50	THR
1	E	57	LEU
1	E	58	VAL
1	E	59	LYS
1	E	76	GLU
2	F	4	LEU
2	F	8	THR
2	F	13	THR
2	F	52	THR
2	F	62	LEU
2	F	74	THR
2	F	75	GLU
2	F	83	VAL
2	F	90	THR
2	F	98	LEU
2	F	147	THR
2	F	152	ASN
1	G	4	ILE
1	G	15	ASP
1	G	19	LYS
1	G	34	LYS
1	G	36	LYS
1	G	37	SER
1	G	51	THR
2	H	13	THR
2	H	25	ARG
2	H	46	GLN
2	H	57	LYS
2	H	64	THR
2	H	68	PRO
2	H	70	LEU
2	H	71	ARG
2	H	76	THR

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Mol	Chain	Res	Type
2	H	79	ILE
2	H	80	GLU
2	H	82	SER
2	H	84	VAL
2	H	90	THR
2	H	91	MET
2	H	95	THR
2	H	98	LEU
2	H	101	THR
2	H	111	THR
2	H	116	SER
2	H	118	THR
2	H	149	PHE
1	I	11	PRO
1	I	12	GLU
1	I	16	LEU
1	I	29	SER
1	I	36	LYS
1	I	37	SER
1	I	41	GLU
1	I	44	LYS
1	I	59	LYS
1	I	60	GLN
2	J	1	MET
2	J	3	LEU
2	J	13	THR
2	J	14	ASP
2	J	28	ASN
2	J	33	HIS
2	J	63	PRO
2	J	64	THR
2	J	74	THR
2	J	75	GLU
2	J	82	SER
2	J	90	THR
2	J	97	ASN
2	J	98	LEU
2	J	101	THR
2	J	104	MET
2	J	108	GLU
2	J	111	THR
2	J	127	VAL

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Mol	Chain	Res	Type
2	J	128	LYS
2	J	134	ASN
2	J	149	PHE
2	J	163	VAL
2	J	164	ILE
2	J	166	LYS
1	K	58	VAL
1	K	59	LYS
1	K	67	ASP
2	L	1	MET
2	L	2	VAL
2	L	3	LEU
2	L	10	ILE
2	L	13	THR
2	L	29	PRO
2	L	31	SER
2	L	42	ARG
2	L	43	ASN
2	L	45	ASP
2	L	46	GLN
2	L	47	GLU
2	L	49	ASN
2	L	50	LEU
2	L	55	LEU
2	L	57	LYS
2	L	59	SER
2	L	70	LEU
2	L	73	ILE
2	L	76	THR
2	L	94	TYR
2	L	95	THR
2	L	98	LEU
2	L	101	THR
2	L	113	GLN
2	L	120	SER
2	L	122	ILE
2	L	154	LYS
1	M	39	GLU
1	M	43	SER
2	N	3	LEU
2	N	4	LEU
2	N	74	THR

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Mol	Chain	Res	Type
2	N	75	GLU
2	N	133	PHE
2	N	134	ASN
2	N	135	MET
2	N	137	ILE
2	N	142	GLU
2	N	157	ARG
2	N	166	LYS
1	O	39	GLU
1	O	43	SER
1	O	75	PHE
2	P	1	MET
2	P	129	PHE
2	P	131	SER
2	P	140	LYS
2	P	154	LYS
2	P	165	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
2	B	49	ASN
2	B	100	HIS
2	B	113	GLN
2	D	5	HIS
2	D	9	HIS
2	D	46	GLN
2	D	134	ASN
2	F	43	ASN
2	F	113	GLN
1	G	45	GLN
2	H	9	HIS
1	I	54	ASN
2	J	5	HIS
2	J	9	HIS
2	J	46	GLN
2	J	97	ASN
2	J	165	GLN
1	K	54	ASN
2	L	9	HIS
2	L	46	GLN

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Mol	Chain	Res	Type
2	L	152	ASN
1	M	54	ASN
2	N	152	ASN
2	P	9	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PX2	F	201	-	35,35,35	0.70	0	38,40,40	1.11	1 (2%)
3	PX2	B	201	-	35,35,35	0.67	0	38,40,40	1.18	3 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX2	F	201	-	-	10/37/37/37	-
3	PX2	B	201	-	-	9/37/37/37	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	201	PX2	C2-O7-C16	-3.63	109.11	117.80
3	B	201	PX2	C2-O7-C16	-2.70	111.33	117.80
3	B	201	PX2	C3-O5-C4	-2.34	108.55	117.12
3	B	201	PX2	O3-P1-O4	-2.19	100.97	106.67

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	201	PX2	C2-C1-O4-P1
3	B	201	PX2	C17-C16-O7-C2
3	F	201	PX2	C5-C4-O5-C3
3	F	201	PX2	O6-C4-O5-C3
3	B	201	PX2	O8-C16-O7-C2
3	B	201	PX2	O6-C4-O5-C3
3	F	201	PX2	C17-C16-O7-C2
3	F	201	PX2	C23-C24-C25-C26
3	B	201	PX2	C5-C4-O5-C3
3	F	201	PX2	O8-C16-O7-C2
3	B	201	PX2	C17-C18-C19-C20
3	F	201	PX2	C1-C2-O7-C16
3	F	201	PX2	C3-C2-O7-C16
3	B	201	PX2	O5-C4-C5-C6
3	F	201	PX2	O7-C16-C17-C18
3	B	201	PX2	O7-C16-C17-C18
3	F	201	PX2	O8-C16-C17-C18
3	B	201	PX2	O8-C16-C17-C18
3	B	201	PX2	O6-C4-C5-C6

There are no ring outliers.

2 monomers are involved in 15 short contacts:

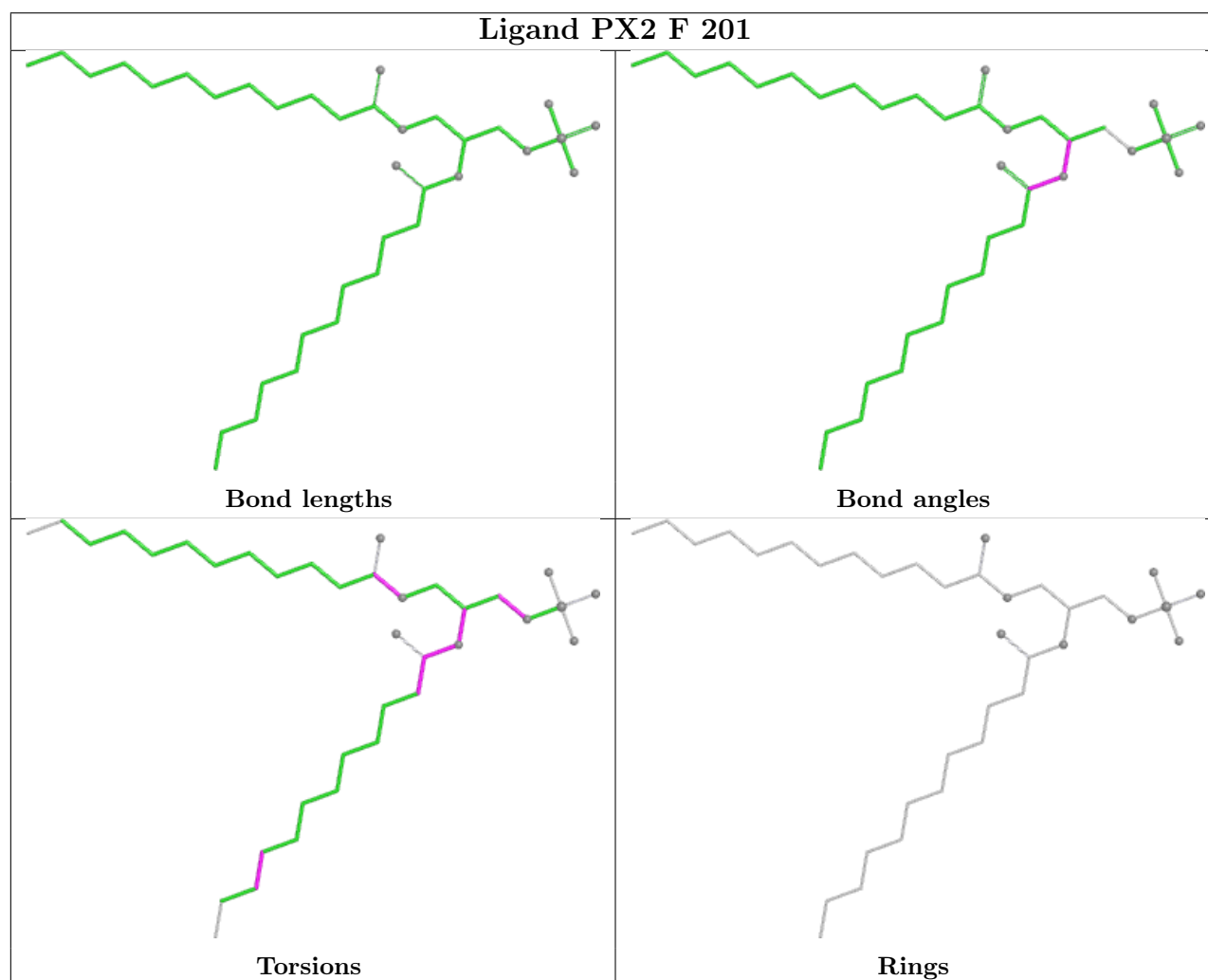
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	201	PX2	7	0

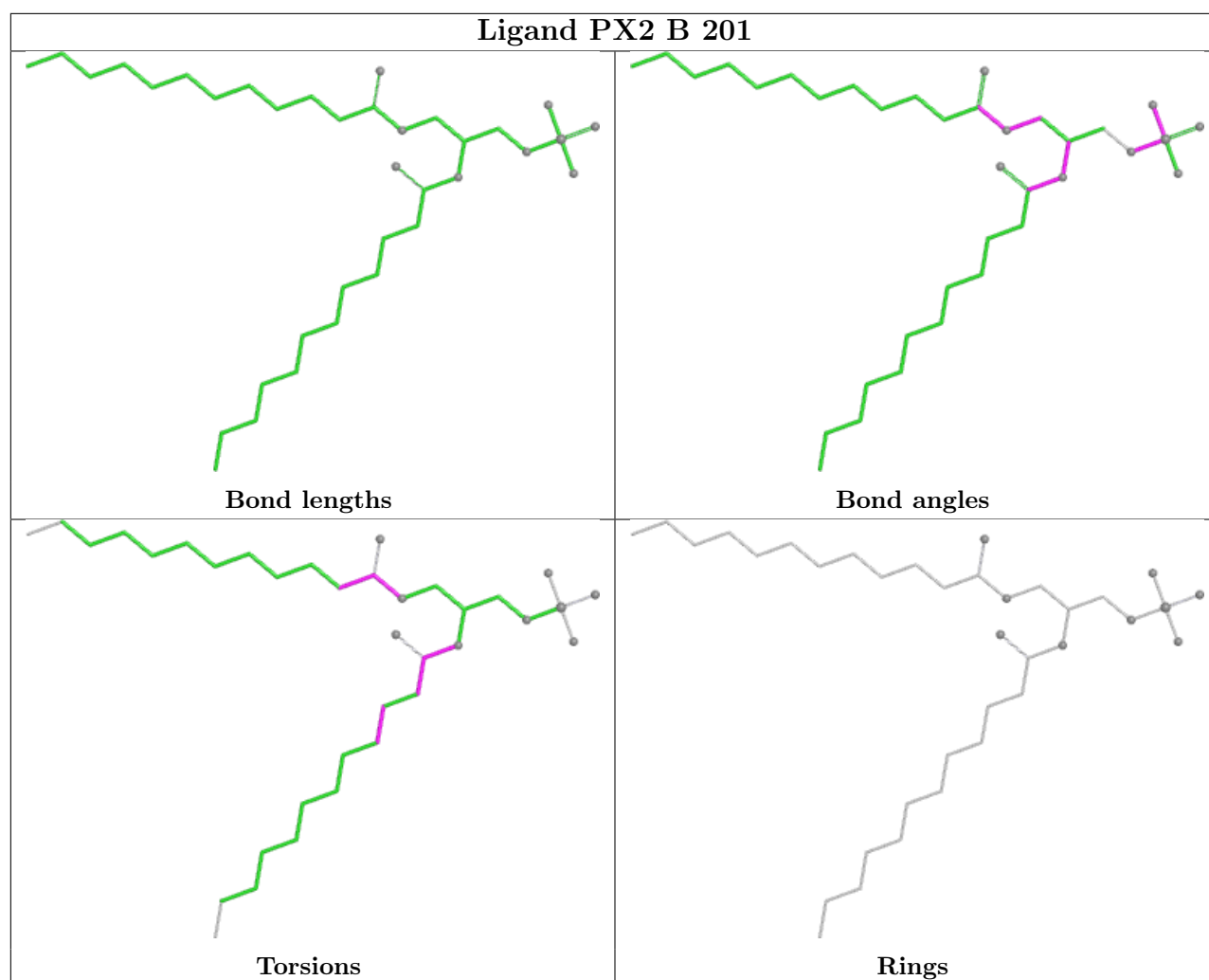
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	201	PX2	8	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	73/81 (90%)	-0.21	0 100 100	44, 64, 100, 113	0
1	C	73/81 (90%)	0.07	2 (2%) 56 36	34, 52, 92, 100	0
1	E	73/81 (90%)	0.19	3 (4%) 41 25	52, 78, 112, 125	0
1	G	73/81 (90%)	0.02	0 100 100	54, 72, 107, 121	0
1	I	73/81 (90%)	0.23	1 (1%) 73 54	69, 93, 117, 126	0
1	K	73/81 (90%)	1.29	11 (15%) 5 4	120, 139, 165, 171	0
1	M	73/81 (90%)	1.04	6 (8%) 17 11	142, 156, 167, 171	0
1	O	68/81 (83%)	1.91	27 (39%) 1 1	193, 208, 216, 216	0
2	B	160/184 (86%)	0.17	4 (2%) 58 39	34, 59, 153, 157	0
2	D	170/184 (92%)	-0.13	1 (0%) 85 73	30, 52, 89, 93	0
2	F	167/184 (90%)	0.02	3 (1%) 67 48	35, 60, 112, 128	0
2	H	162/184 (88%)	0.29	6 (3%) 45 28	42, 70, 142, 183	0
2	J	169/184 (91%)	0.07	2 (1%) 76 58	46, 64, 107, 117	0
2	L	169/184 (91%)	0.31	5 (2%) 52 33	42, 76, 129, 147	0
2	N	157/184 (85%)	1.31	42 (26%) 1 1	43, 131, 150, 160	0
2	P	159/184 (86%)	1.80	66 (41%) 0 1	54, 189, 207, 213	0
All	All	1892/2120 (89%)	0.49	179 (9%) 14 9	30, 75, 200, 216	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	79	ILE	8.9
2	P	55	LEU	8.2
1	O	38	VAL	5.9
2	P	78	ILE	5.8
2	P	44	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
2	P	53	THR	5.5
2	P	98	LEU	5.5
1	O	62	ILE	5.3
2	P	56	LEU	5.2
1	O	61	GLY	5.1
2	N	26	TYR	5.1
1	I	4	ILE	4.9
1	M	38	VAL	4.8
2	P	18	VAL	4.6
1	O	66	LEU	4.6
2	P	82	SER	4.5
2	N	129	PHE	4.5
2	P	73	ILE	4.3
1	K	51	THR	4.2
1	M	4	ILE	4.2
2	N	39	THR	4.2
2	P	81	VAL	4.2
2	F	66	VAL	4.1
2	N	78	ILE	4.1
2	P	94	TYR	4.0
2	P	11	PHE	3.9
2	N	48	GLY	3.9
2	N	27	PRO	3.8
2	N	61	LYS	3.8
2	B	65	TRP	3.8
1	K	47	TYR	3.8
2	P	5	HIS	3.7
2	P	97	ASN	3.7
2	L	4	LEU	3.7
2	N	24	ASN	3.7
2	P	92	LYS	3.6
2	P	26	TYR	3.6
2	P	83	VAL	3.5
2	P	106	VAL	3.5
1	K	55	ALA	3.5
2	P	45	ASP	3.5
2	P	127	VAL	3.4
2	P	40	ILE	3.4
2	P	124	ASP	3.3
2	P	7	SER	3.3
2	B	159	GLY	3.3
2	P	10	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	N	44	VAL	3.3
2	N	30	TYR	3.3
1	E	40	ASN	3.3
2	P	52	THR	3.2
2	P	32	PRO	3.2
2	P	1	MET	3.2
2	P	76	THR	3.2
1	M	5	MET	3.1
2	P	46	GLN	3.1
2	P	29	PRO	3.1
2	P	33	HIS	3.1
2	P	6	LYS	3.1
2	P	12	PRO	3.1
2	P	43	ASN	3.0
2	N	114	PHE	3.0
2	N	94	TYR	3.0
2	P	95	THR	3.0
2	B	66	VAL	3.0
1	O	9	PHE	3.0
2	P	74	THR	3.0
2	P	4	LEU	2.9
1	O	11	PRO	2.9
2	L	65	TRP	2.9
1	K	38	VAL	2.9
2	H	109	TYR	2.9
2	N	37	ILE	2.9
2	P	8	THR	2.9
2	P	41	SER	2.8
1	O	39	GLU	2.8
2	H	160	MET	2.8
1	O	28	TYR	2.8
2	H	5	HIS	2.8
1	O	69	ALA	2.8
2	N	21	ALA	2.8
1	O	71	GLU	2.8
2	N	11	PHE	2.7
1	K	62	ILE	2.7
1	O	57	LEU	2.7
1	K	4	ILE	2.7
2	N	6	LYS	2.7
1	O	36	LYS	2.7
1	O	43	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	N	98	LEU	2.7
2	N	124	ASP	2.6
2	P	13	THR	2.6
2	P	77	TRP	2.6
2	B	137	ILE	2.6
1	O	60	GLN	2.6
2	H	159	GLY	2.6
2	N	119	SER	2.6
2	N	102	GLY	2.6
2	P	58	LYS	2.6
2	N	10	ILE	2.5
2	N	116	SER	2.5
2	P	35	LEU	2.5
1	O	29	SER	2.5
1	K	48	ALA	2.5
2	P	129	PHE	2.5
2	P	72	GLY	2.5
2	D	119	SER	2.5
1	K	9	PHE	2.5
1	O	40	ASN	2.5
1	O	74	PRO	2.5
2	N	163	VAL	2.5
1	M	32	PHE	2.4
1	K	61	GLY	2.4
2	P	80	GLU	2.4
1	O	16	LEU	2.4
2	N	5	HIS	2.4
1	C	59	LYS	2.4
2	H	152	ASN	2.4
1	K	10	ALA	2.4
2	N	22	PHE	2.4
2	P	23	PHE	2.3
1	O	58	VAL	2.3
1	O	31	LYS	2.3
2	N	112	TYR	2.3
2	P	17	SER	2.3
2	N	109	TYR	2.3
2	F	4	LEU	2.3
2	P	50	LEU	2.3
1	O	19	LYS	2.3
2	N	58	LYS	2.3
2	P	38	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	P	126	ARG	2.3
2	P	99	ASP	2.3
2	L	72	GLY	2.2
2	N	29	PRO	2.2
2	P	27	PRO	2.2
2	N	50	LEU	2.2
1	O	75	PHE	2.2
1	O	15	ASP	2.2
2	J	167	LEU	2.2
1	E	75	PHE	2.2
2	P	61	LYS	2.2
2	P	112	TYR	2.2
2	N	106	VAL	2.2
2	L	76	THR	2.2
2	N	103	ILE	2.2
2	N	56	LEU	2.2
2	F	63	PRO	2.2
2	P	128	LYS	2.2
2	J	129	PHE	2.2
2	N	54	ARG	2.2
2	P	54	ARG	2.2
1	O	27	TRP	2.2
2	N	25	ARG	2.2
2	N	38	ASP	2.2
2	P	9	HIS	2.2
2	N	8	THR	2.1
1	M	55	ALA	2.1
2	N	100	HIS	2.1
2	N	52	THR	2.1
2	P	47	GLU	2.1
2	P	84	VAL	2.1
2	L	5	HIS	2.1
2	P	39	THR	2.1
2	P	30	TYR	2.1
1	O	70	ARG	2.1
2	N	117	ALA	2.1
1	M	75	PHE	2.1
1	C	62	ILE	2.1
1	E	62	ILE	2.1
2	P	22	PHE	2.1
1	K	49	TYR	2.0
1	O	10	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	O	14	THR	2.0
2	N	79	ILE	2.0
2	P	37	ILE	2.0
2	H	154	LYS	2.0
2	P	34	VAL	2.0
2	N	40	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

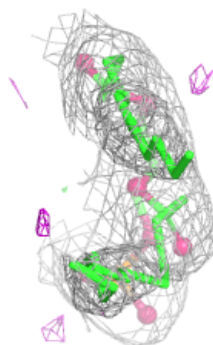
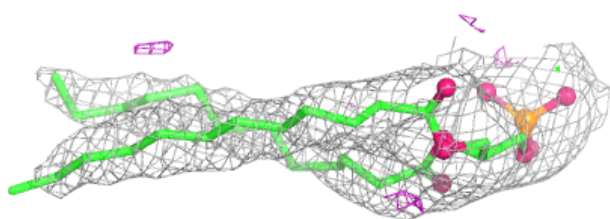
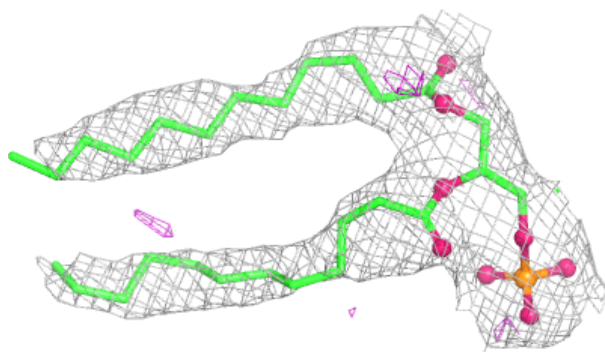
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PX2	B	201	36/36	0.93	0.13	44,55,62,63	0
3	PX2	F	201	36/36	0.94	0.17	54,63,76,78	0

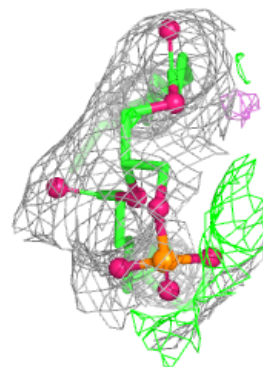
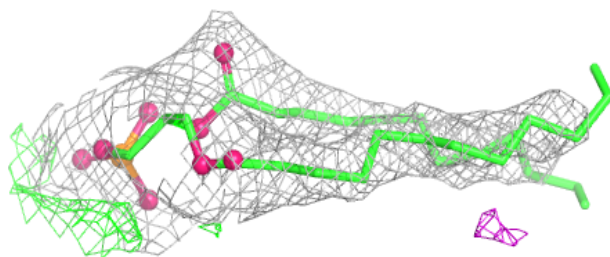
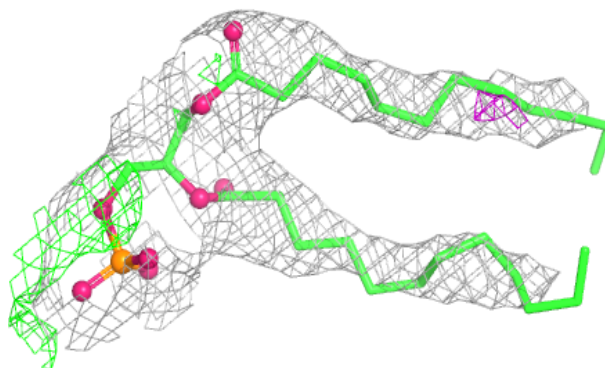
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PX2 B 201:

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

**Electron density around PX2 F 201:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.