



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 04:24 PM JST

PDB ID : 7CHL
Title : Crystal structure of hybrid Arabinose isomerase AI-10
Authors : Cao, T.P.; Dhanasingh, I.; Sung, J.Y.; Shin, S.M.; Lee, D.W.; Lee, S.H.
Deposited on : 2020-07-06
Resolution : 3.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

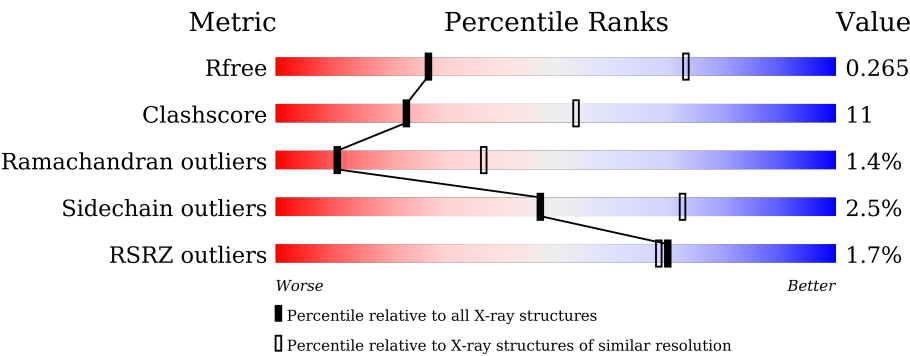
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	498	<div><div>2%</div><div>69%</div><div>30%</div><div>.</div></div>
1	B	498	<div><div>%</div><div>72%</div><div>26%</div><div>.</div></div>
1	C	498	<div><div>2%</div><div>69%</div><div>30%</div><div>.</div></div>
1	D	498	<div><div>2%</div><div>72%</div><div>26%</div><div>.</div></div>
1	E	498	<div><div>%</div><div>69%</div><div>28%</div><div>.</div></div>
1	F	498	<div><div>%</div><div>75%</div><div>24%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	G	498	<div><div></div><div>3%</div><div>71%</div><div>28%</div><div></div></div>
1	H	498	<div><div></div><div>2%</div><div>74%</div><div>23%</div><div></div></div>
1	I	498	<div><div></div><div>%</div><div>66%</div><div>32%</div><div></div></div>
1	J	498	<div><div></div><div>%</div><div>73%</div><div>27%</div><div></div></div>
1	K	498	<div><div></div><div>2%</div><div>72%</div><div>26%</div><div></div></div>
1	L	498	<div><div></div><div>3%</div><div>71%</div><div>26%</div><div></div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 47178 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 Hybrid Arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	1	0
			3945	2503	699	721	22			
1	B	497	Total	C	N	O	S	0	0	0
			3922	2491	691	718	22			
1	C	498	Total	C	N	O	S	0	0	0
			3934	2497	695	720	22			
1	D	498	Total	C	N	O	S	0	0	0
			3934	2497	695	720	22			
1	E	497	Total	C	N	O	S	0	0	0
			3922	2491	691	718	22			
1	F	496	Total	C	N	O	S	0	0	0
			3914	2486	690	717	21			
1	G	498	Total	C	N	O	S	0	0	0
			3934	2497	695	720	22			
1	H	497	Total	C	N	O	S	0	0	0
			3922	2491	691	718	22			
1	I	498	Total	C	N	O	S	0	0	0
			3934	2497	695	720	22			
1	J	498	Total	C	N	O	S	0	0	0
			3934	2497	695	720	22			
1	K	498	Total	C	N	O	S	0	0	0
			3933	2497	695	719	22			
1	L	496	Total	C	N	O	S	0	0	0
			3914	2486	690	717	21			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0
2	E	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0
2	G	1	Total 1	Mn 1	0	0
2	H	1	Total 1	Mn 1	0	0
2	I	1	Total 1	Mn 1	0	0
2	J	1	Total 1	Mn 1	0	0
2	K	1	Total 1	Mn 1	0	0
2	L	1	Total 1	Mn 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0
3	E	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0
3	G	1	Total 1	Na 1	0	0
3	H	1	Total 1	Na 1	0	0
3	I	1	Total 1	Na 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total 1	Na 1	0	0
3	K	1	Total 1	Na 1	0	0
3	L	1	Total 1	Na 1	0	0

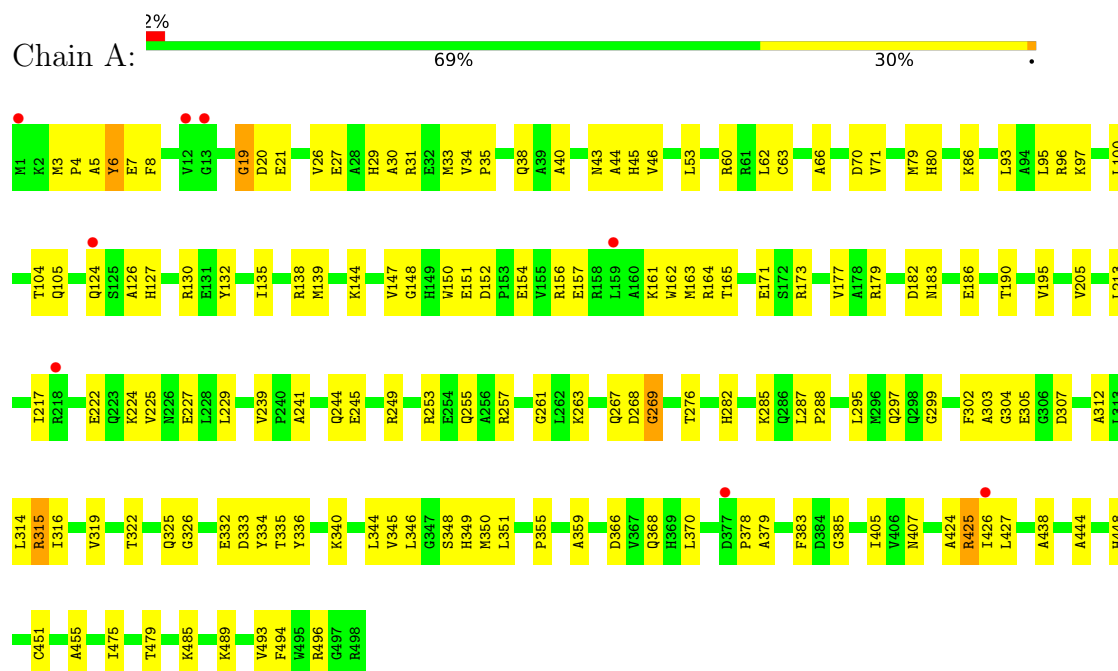
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	B	2	Total 2	O 2	0	0
4	C	1	Total 1	O 1	0	0
4	D	1	Total 1	O 1	0	0
4	F	1	Total 1	O 1	0	0
4	G	1	Total 1	O 1	0	0
4	I	2	Total 2	O 2	0	0
4	J	1	Total 1	O 1	0	0
4	K	1	Total 1	O 1	0	0
4	L	1	Total 1	O 1	0	0

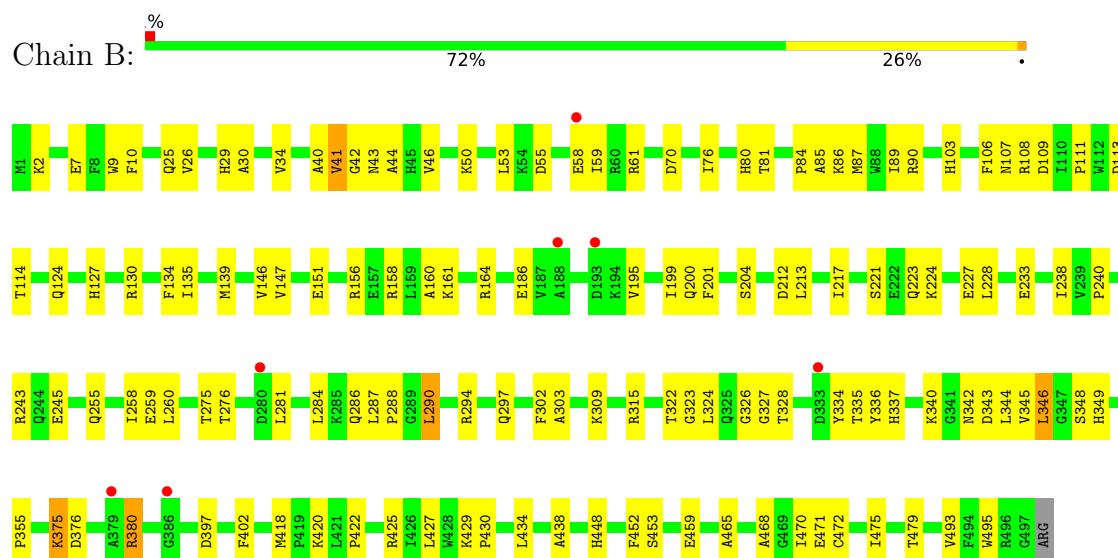
3 Residue-property plots [i](#)

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.

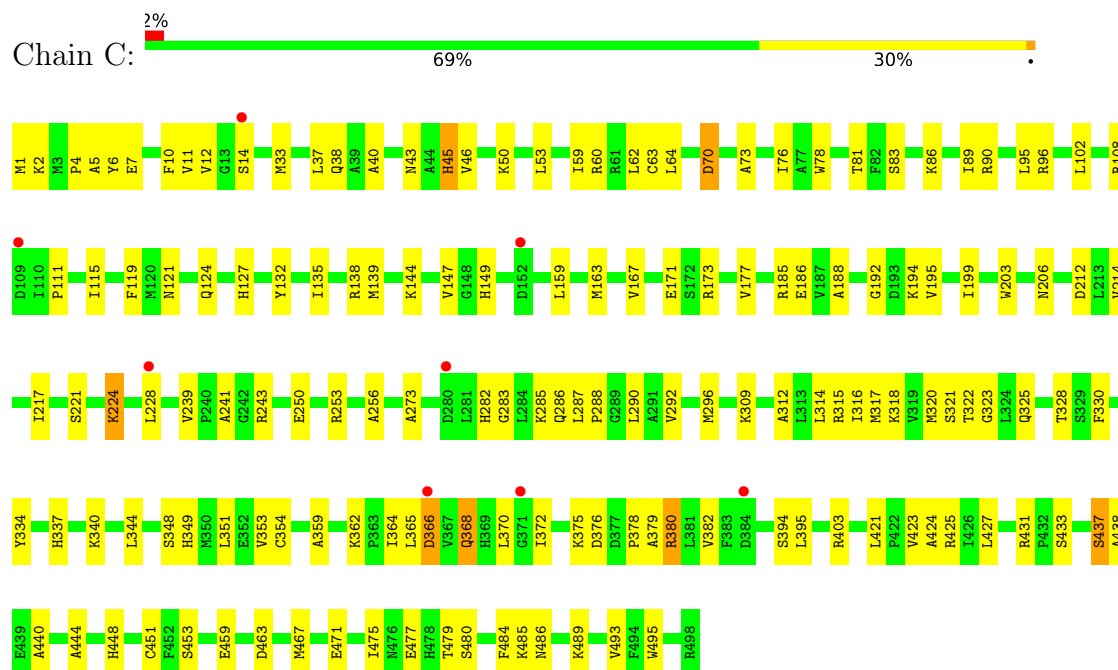
• Molecule 1: Hybrid Arabinose isomerase



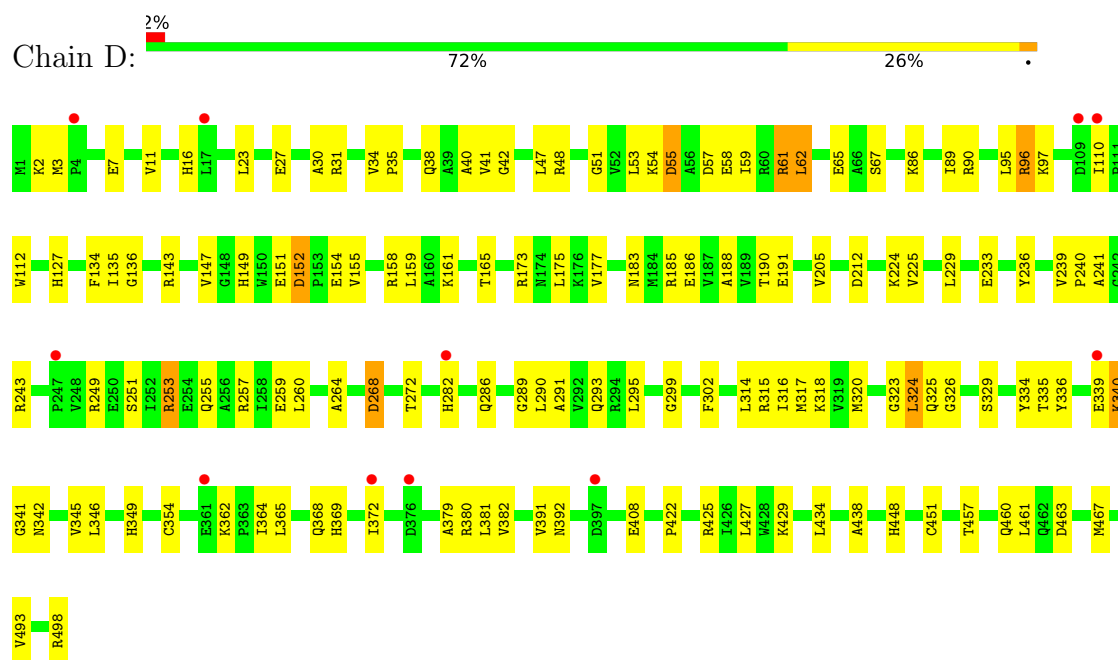
• Molecule 1: Hybrid Arabinose isomerase



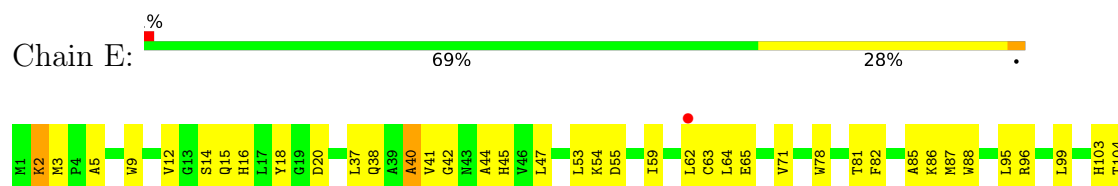
• Molecule 1: Hybrid Arabinose isomerase



• Molecule 1: Hybrid Arabinose isomerase

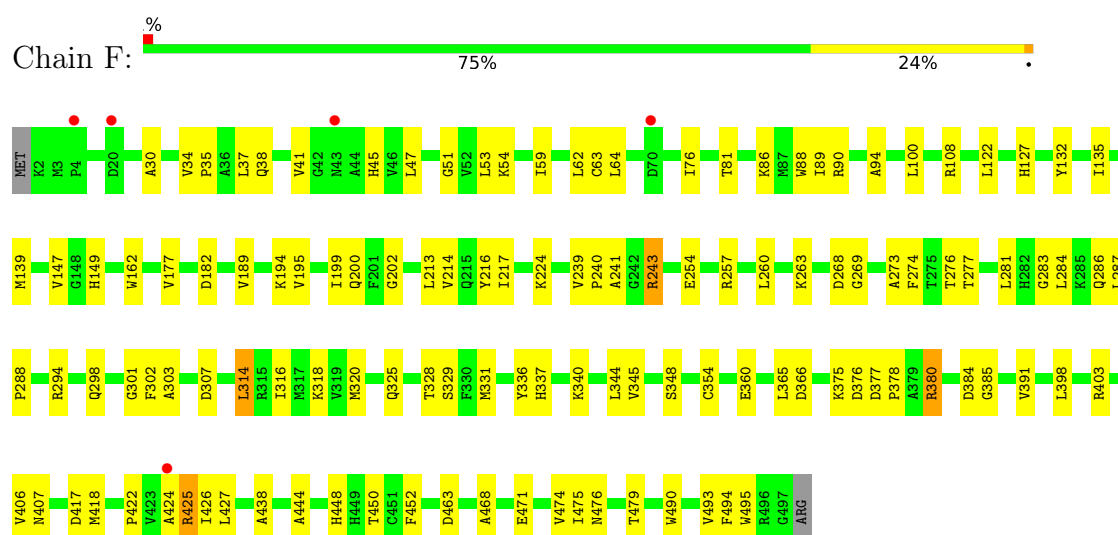


• Molecule 1: Hybrid Arabinose isomerase

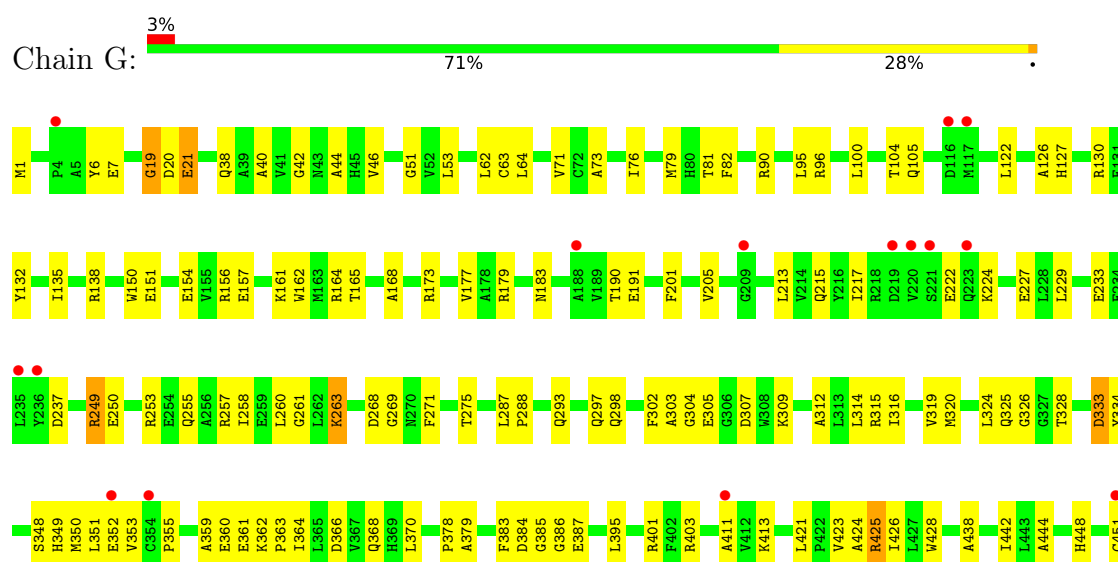




● Molecule 1: Hybrid Arabinose isomerase

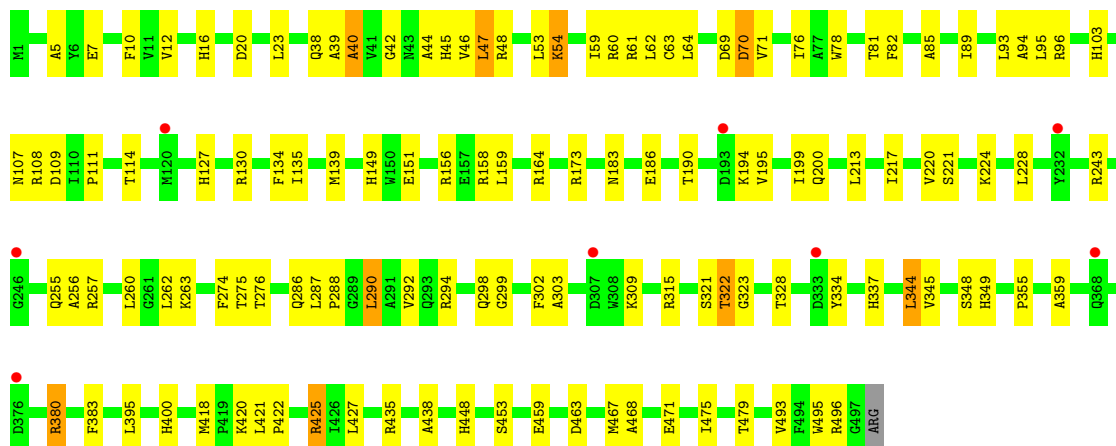
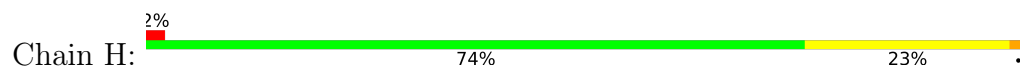


● Molecule 1: Hybrid Arabinose isomerase

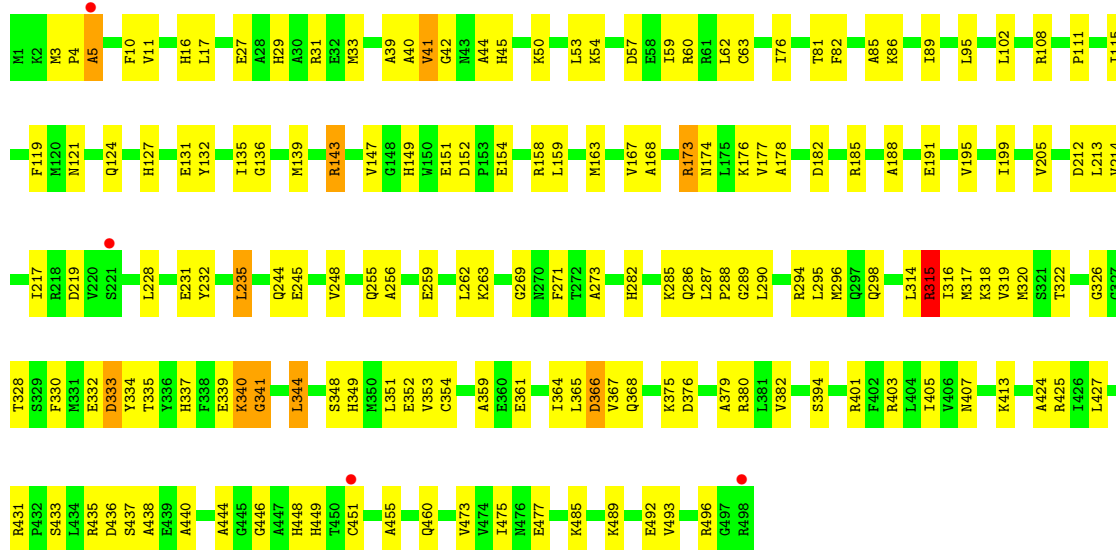




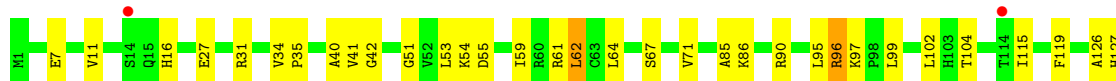
• Molecule 1: Hybrid Arabinose isomerase

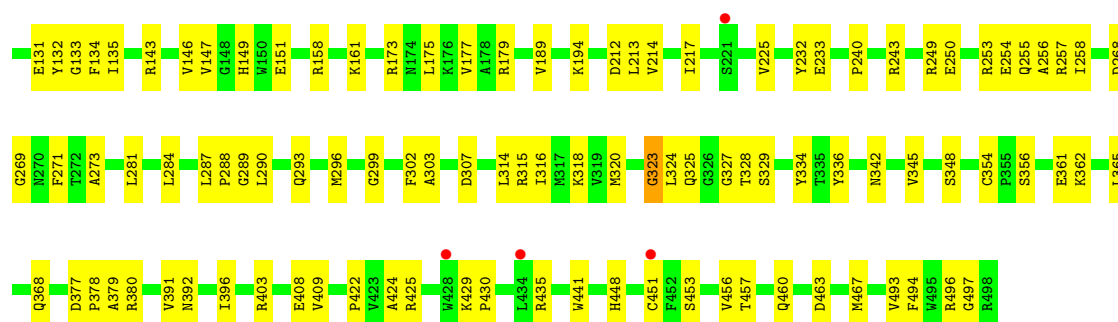


• Molecule 1: Hybrid Arabinose isomerase

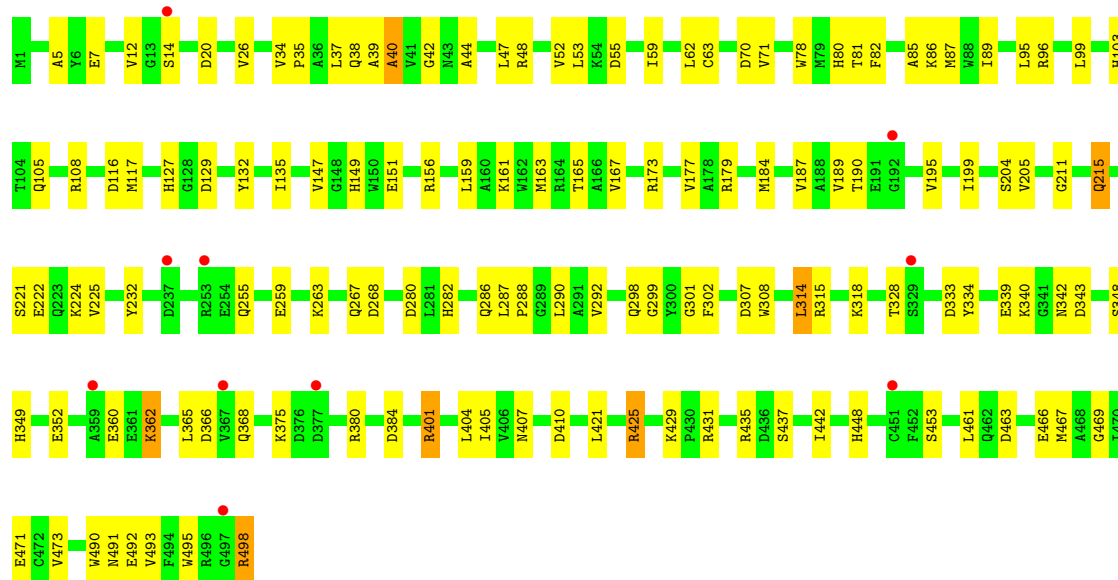
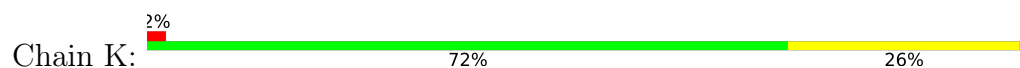


• Molecule 1: Hybrid Arabinose isomerase

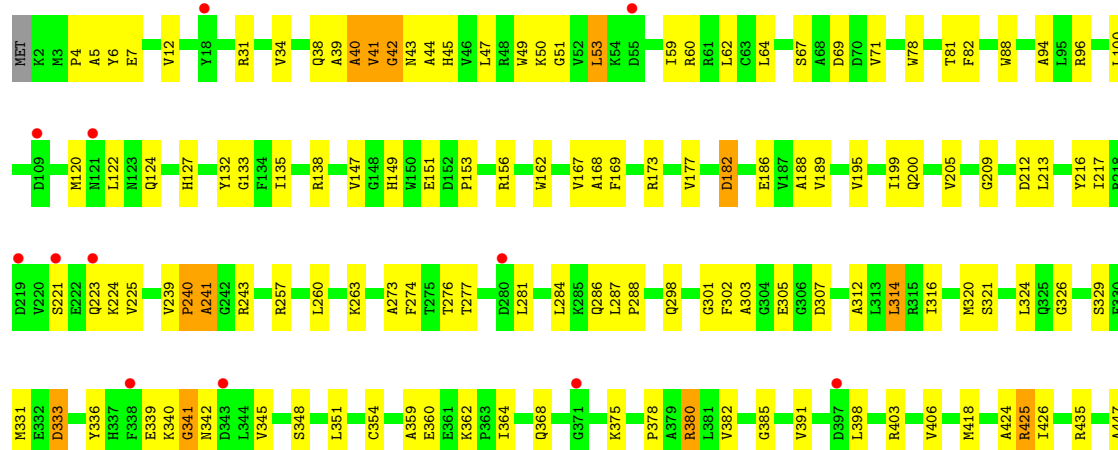




● Molecule 1: Hybrid Arabinose isomerase



● Molecule 1: Hybrid Arabinose isomerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	152.09Å 164.30Å 151.97Å 90.00° 119.92° 90.00°	Depositor
Resolution (Å)	30.54 – 3.40 30.54 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.3 (30.54-3.40) 95.3 (30.54-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.00 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.208 , 0.264 0.208 , 0.265	Depositor DCC
R_{free} test set	4249 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , -7.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.186 for l,k,-h-l 0.186 for -h-l,k,h 0.448 for -h-l,-k,l 0.178 for h,-k,-h-l 0.196 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47178	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.88% 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: MN, NA

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	0.26	0/4037	0.50	0/5460
1	B	0.27	0/4014	0.50	1/5432 (0.0%)
1	C	0.28	0/4026	0.50	0/5446
1	D	0.27	0/4026	0.50	0/5446
1	E	0.27	0/4014	0.53	3/5432 (0.1%)
1	F	0.27	0/4006	0.53	1/5422 (0.0%)
1	G	0.27	0/4026	0.52	0/5446
1	H	0.27	0/4014	0.50	3/5432 (0.1%)
1	I	0.28	0/4026	0.53	3/5446 (0.1%)
1	J	0.27	0/4026	0.49	0/5446
1	K	0.27	0/4025	0.52	1/5446 (0.0%)
1	L	0.27	0/4006	0.55	2/5422 (0.0%)
All	All	0.27	0/48246	0.51	14/65276 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	314	LEU	CA-CB-CG	8.32	134.44	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	314	LEU	CA-CB-CG	7.99	133.67	115.30
1	E	314	LEU	CA-CB-CG	7.76	133.15	115.30
1	L	314	LEU	CA-CB-CG	7.75	133.12	115.30
1	I	235	LEU	CA-CB-CG	6.61	130.49	115.30
1	E	290	LEU	CA-CB-CG	5.70	128.42	115.30
1	L	42	GLY	N-CA-C	-5.68	98.91	113.10
1	H	344	LEU	CA-CB-CG	5.64	128.27	115.30
1	B	290	LEU	CA-CB-CG	5.60	128.18	115.30
1	H	47	LEU	CA-CB-CG	5.47	127.87	115.30
1	H	290	LEU	CA-CB-CG	5.40	127.73	115.30
1	I	315	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	I	344	LEU	CA-CB-CG	5.24	127.36	115.30
1	E	323	GLY	N-CA-C	-5.12	100.30	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	ASN	Peptide
1	E	323	GLY	Peptide
1	F	38	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3945	0	3862	97	0
1	B	3922	0	3837	95	0
1	C	3934	0	3850	103	0
1	D	3934	0	3850	99	0
1	E	3922	0	3837	105	0
1	F	3914	0	3825	86	0
1	G	3934	0	3850	96	0
1	H	3922	0	3837	84	0
1	I	3934	0	3850	113	0
1	J	3934	0	3850	86	0
1	K	3933	0	3850	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3914	0	3825	102	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	I	2	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
All	All	47178	0	46123	1057	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 11.

All (1057) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:GLU:OE2	1:D:48:ARG:NH2	1.86	1.09
1:F:286:GLN:HE21	1:F:378:PRO:HA	1.29	0.97
1:D:7:GLU:OE1	1:D:48:ARG:NE	1.97	0.97
1:D:7:GLU:CD	1:D:48:ARG:NH2	2.18	0.95
1:K:53:LEU:HB3	1:K:59:ILE:HG22	1.48	0.93
1:A:494:PHE:HA	1:D:493:VAL:HG11	1.50	0.93
1:E:53:LEU:HB3	1:E:59:ILE:HG22	1.51	0.92
1:D:7:GLU:OE1	1:D:48:ARG:NH2	2.03	0.92
1:E:255:GLN:HG2	1:E:290:LEU:HB3	1.53	0.91
1:D:7:GLU:OE1	1:D:48:ARG:CZ	2.19	0.90
1:A:493:VAL:HG21	1:F:494:PHE:HA	1.53	0.89
1:G:494:PHE:HA	1:J:493:VAL:HG11	1.57	0.86
1:J:127:HIS:HB2	1:L:448:HIS:HB2	1.57	0.86
1:A:326:GLY:HA3	1:A:455:ALA:HB2	1.56	0.86
1:L:38:GLN:H	1:L:39:ALA:HB3	1.42	0.84
1:K:401:ARG:NH2	1:K:471:GLU:OE1	2.11	0.83
1:I:448:HIS:HB2	1:K:127:HIS:HB2	1.61	0.82
1:G:493:VAL:HG21	1:L:494:PHE:HA	1.61	0.82
1:C:448:HIS:HB2	1:E:127:HIS:HB2	1.61	0.81
1:E:401:ARG:NH2	1:E:471:GLU:OE1	2.13	0.81
1:F:37:LEU:O	1:F:41:VAL:HB	1.82	0.81
1:D:134:PHE:CD2	1:F:189:VAL:HG22	2.17	0.79
1:I:496:ARG:HH22	1:J:497:GLY:HA2	1.46	0.79
1:H:255:GLN:HG2	1:H:290:LEU:HB3	1.62	0.79
1:C:475:ILE:HG13	1:C:479:THR:HG21	1.63	0.79
1:K:255:GLN:HG2	1:K:290:LEU:HB3	1.64	0.78
1:D:229:LEU:HD21	1:D:249:ARG:HE	1.44	0.78
1:G:127:HIS:HB2	1:J:448:HIS:HB2	1.66	0.78
1:A:34:VAL:HG23	1:A:35:PRO:HD3	1.67	0.77
1:F:286:GLN:NE2	1:F:378:PRO:HA	1.98	0.77
1:C:60:ARG:O	1:C:64:LEU:CD1	2.33	0.77
1:L:385:GLY:HA3	1:L:426:ILE:HG13	1.65	0.77
1:B:127:HIS:HB2	1:E:448:HIS:HB2	1.67	0.76
1:D:323:GLY:HA2	1:D:324:LEU:HB2	1.67	0.76
1:D:134:PHE:CG	1:F:189:VAL:HG22	2.20	0.76
1:B:41:VAL:HG13	1:B:160:ALA:HB1	1.66	0.76
1:K:362:LYS:H	1:K:362:LYS:HD2	1.49	0.76
1:I:351:LEU:HD12	1:I:352:GLU:HG3	1.67	0.75
1:B:448:HIS:HB2	1:C:127:HIS:HB2	1.68	0.75
1:C:286:GLN:HG2	1:C:376:ASP:HB2	1.69	0.74
1:B:380:ARG:NH1	1:B:422:PRO:O	2.21	0.74
1:H:321:SER:O	1:H:323:GLY:N	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60[B]:ARG:NH1	1:C:70:ASP:OD2	2.20	0.73
1:J:318:LYS:NZ	1:J:328:THR:HG23	2.02	0.73
1:B:255:GLN:HG2	1:B:290:LEU:HB3	1.70	0.73
1:K:40:ALA:HB2	1:K:156:ARG:HH11	1.54	0.73
1:A:150:TRP:O	1:A:156:ARG:NH1	2.22	0.73
1:H:38:GLN:HG2	1:H:47:LEU:HD23	1.71	0.73
1:E:59:ILE:HD11	1:E:88:TRP:HA	1.71	0.73
1:B:158:ARG:NH1	1:B:459:GLU:OE2	2.22	0.72
1:C:337:HIS:HB3	1:C:344:LEU:HB3	1.71	0.72
1:H:127:HIS:HB2	1:K:448:HIS:HB2	1.70	0.72
1:C:440:ALA:HB3	1:C:475:ILE:HD12	1.72	0.72
1:B:340:LYS:NZ	1:I:361:GLU:OE2	2.19	0.71
1:A:127:HIS:HB2	1:D:448:HIS:HB2	1.73	0.71
1:J:134:PHE:CD2	1:L:189:VAL:HG22	2.26	0.71
1:E:249:ARG:HA	1:E:252:ILE:HD12	1.72	0.71
1:C:348:SER:OG	1:C:424:ALA:O	2.08	0.71
1:F:53:LEU:HD13	1:F:59:ILE:HD13	1.73	0.70
1:H:418:MET:HG2	1:I:115:ILE:HD11	1.72	0.70
1:D:302:PHE:H	1:D:314:LEU:HD23	1.55	0.70
1:H:448:HIS:HB2	1:I:127:HIS:HB2	1.73	0.70
1:J:16:HIS:CE1	1:J:54:LYS:HD2	2.26	0.70
1:C:60:ARG:O	1:C:64:LEU:HD12	1.91	0.70
1:D:7:GLU:CD	1:D:48:ARG:CZ	2.59	0.70
1:A:366:ASP:OD2	1:A:368:GLN:NE2	2.24	0.70
1:J:302:PHE:H	1:J:314:LEU:HD23	1.57	0.69
1:B:418:MET:HG2	1:C:115:ILE:HD11	1.72	0.69
1:E:255:GLN:OE1	1:E:286:GLN:NE2	2.26	0.69
1:G:293:GLN:NE2	1:G:351:LEU:O	2.24	0.69
1:E:255:GLN:HE22	1:E:288:PRO:HA	1.58	0.69
1:F:418:MET:HB2	1:F:425:ARG:HH21	1.56	0.69
1:E:252:ILE:HG12	1:E:365:LEU:HD11	1.75	0.68
1:H:224:LYS:CE	1:H:260:LEU:HD22	2.24	0.68
1:I:353:VAL:HG11	1:I:424:ALA:HB3	1.74	0.68
1:C:321:SER:O	1:C:323:GLY:N	2.25	0.68
1:E:232:TYR:OH	1:E:259:GLU:OE1	2.12	0.68
1:A:297:GLN:HG3	1:A:355:PRO:HG2	1.74	0.68
1:K:42:GLY:O	1:K:44:ALA:N	2.22	0.68
1:K:37:LEU:HD12	1:K:47:LEU:HD11	1.76	0.67
1:J:225:VAL:HG21	1:J:257:ARG:HG3	1.76	0.67
1:E:37:LEU:HD12	1:E:47:LEU:HD11	1.76	0.67
1:G:448:HIS:HB2	1:L:127:HIS:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:418:MET:HB2	1:L:425:ARG:HH21	1.59	0.67
1:C:366:ASP:O	1:C:379:ALA:HA	1.95	0.67
1:C:440:ALA:HB3	1:C:475:ILE:CD1	2.24	0.66
1:E:40:ALA:HB2	1:E:156:ARG:HH11	1.59	0.66
1:H:220:VAL:HG21	1:H:257:ARG:HG2	1.75	0.66
1:K:63:CYS:HB2	1:K:95:LEU:HB2	1.77	0.66
1:G:363:PRO:HB3	1:G:383:PHE:HB3	1.77	0.66
1:I:255:GLN:HG3	1:I:379:ALA:HB3	1.77	0.66
1:K:343:ASP:OD2	1:K:435:ARG:NH2	2.28	0.66
1:A:448:HIS:HB2	1:F:127:HIS:HB2	1.78	0.66
1:H:263:LYS:NZ	1:H:298:GLN:OE1	2.27	0.66
1:F:53:LEU:HD23	1:F:62:LEU:HD22	1.76	0.66
1:C:53:LEU:HD13	1:C:59:ILE:HA	1.78	0.66
1:B:111:PRO:HB2	1:B:114:THR:HG22	1.77	0.66
1:D:362:LYS:H	1:D:362:LYS:HD2	1.61	0.65
1:I:76:ILE:HD11	1:I:102:LEU:HD22	1.79	0.65
1:C:486:ASN:HA	1:C:489:LYS:HD2	1.78	0.65
1:K:302:PHE:H	1:K:314:LEU:HD11	1.62	0.65
1:G:255:GLN:HG3	1:G:379:ALA:HB3	1.77	0.65
1:B:53:LEU:HD12	1:B:59:ILE:HA	1.79	0.65
1:K:255:GLN:NE2	1:K:286:GLN:OE1	2.29	0.65
1:B:348:SER:OG	1:B:349:HIS:N	2.30	0.64
1:E:179:ARG:HD3	1:E:308:TRP:HB3	1.79	0.64
1:I:403:ARG:NH1	1:I:444:ALA:O	2.30	0.64
1:K:222:GLU:O	1:K:225:VAL:HG22	1.97	0.64
1:D:7:GLU:CD	1:D:48:ARG:HH21	1.99	0.64
1:H:70:ASP:OD2	1:L:60:ARG:NH2	2.30	0.64
1:I:177:VAL:HG22	1:I:273:ALA:HB3	1.80	0.64
1:H:337:HIS:HB3	1:H:344:LEU:HB3	1.80	0.64
1:G:297:GLN:HG3	1:G:355:PRO:HG2	1.78	0.64
1:B:328:THR:HA	1:B:452:PHE:O	1.97	0.64
1:J:396:ILE:HG22	1:J:403:ARG:HB3	1.79	0.64
1:D:7:GLU:OE2	1:D:48:ARG:CZ	2.46	0.64
1:E:103:HIS:HB3	1:E:147:VAL:HG22	1.80	0.64
1:H:344:LEU:HD11	1:H:427:LEU:HD23	1.80	0.64
1:A:351:LEU:HD11	1:A:370:LEU:HD22	1.79	0.63
1:H:380:ARG:NH1	1:H:422:PRO:O	2.31	0.63
1:K:221:SER:HB3	1:K:224:LYS:HD3	1.79	0.63
1:C:60:ARG:O	1:C:64:LEU:HD13	1.97	0.63
1:J:177:VAL:HG22	1:J:273:ALA:HB3	1.80	0.63
1:J:95:LEU:HD13	1:J:97:LYS:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:99:LEU:HD23	1:J:143:ARG:HG2	1.79	0.63
1:J:296:MET:O	1:J:318:LYS:HE2	1.98	0.63
1:J:254:GLU:O	1:J:258:ILE:HG12	1.99	0.63
1:B:85:ALA:HB1	1:B:135:ILE:HG13	1.81	0.63
1:E:368:GLN:HB3	1:E:380:ARG:NH2	2.14	0.63
1:C:76:ILE:HD12	1:C:159:LEU:HD21	1.80	0.62
1:A:96:ARG:O	1:A:173:ARG:NH2	2.32	0.62
1:H:111:PRO:HB2	1:H:114:THR:HG22	1.80	0.62
1:I:315:ARG:HG2	1:I:315:ARG:HH21	1.63	0.62
1:I:53:LEU:HD13	1:I:59:ILE:HA	1.81	0.62
1:L:38:GLN:OE1	1:L:47:LEU:N	2.29	0.62
1:F:302:PHE:H	1:F:314:LEU:HD11	1.65	0.62
1:G:63:CYS:HB3	1:G:95:LEU:HB2	1.80	0.62
1:C:50:LYS:HG3	1:C:62:LEU:HD11	1.81	0.62
1:D:27:GLU:OE2	1:D:31:ARG:NH2	2.32	0.62
1:G:237:ASP:HB2	1:G:364:ILE:HG22	1.81	0.62
1:H:328:THR:HG23	1:H:453:SER:HB2	1.81	0.62
1:J:362:LYS:H	1:J:362:LYS:HD2	1.65	0.62
1:A:161:LYS:HD2	1:A:164:ARG:HH12	1.65	0.62
1:D:255:GLN:HG3	1:D:379:ALA:HB3	1.82	0.61
1:E:421:LEU:HD23	1:E:425:ARG:HD3	1.82	0.61
1:G:150:TRP:O	1:G:156:ARG:NH1	2.33	0.61
1:F:59:ILE:HG21	1:F:88:TRP:HA	1.82	0.61
1:J:299:GLY:O	1:J:315:ARG:NH1	2.33	0.61
1:E:37:LEU:HD13	1:E:37:LEU:O	2.00	0.61
1:C:325:GLN:N	1:C:325:GLN:OE1	2.34	0.61
1:D:154:GLU:OE2	1:D:158:ARG:NH2	2.34	0.61
1:H:107:ASN:ND2	1:H:109:ASP:O	2.33	0.61
1:K:368:GLN:HB3	1:K:380:ARG:NH2	2.15	0.60
1:I:296:MET:HE3	1:I:314:LEU:HD11	1.82	0.60
1:K:53:LEU:HD11	1:K:62:LEU:HG	1.83	0.60
1:K:161:LYS:O	1:K:165:THR:HG23	2.01	0.60
1:A:224:LYS:O	1:A:227:GLU:HG2	2.01	0.60
1:A:38:GLN:NE2	1:A:46:VAL:HA	2.16	0.60
1:F:177:VAL:HG22	1:F:273:ALA:HB3	1.82	0.60
1:D:290:LEU:HD22	1:D:365:LEU:HD21	1.83	0.60
1:G:161:LYS:HD2	1:G:164:ARG:HH12	1.67	0.60
1:L:4:PRO:O	1:L:6:TYR:N	2.35	0.60
1:B:402:PHE:HB3	1:B:470:ILE:HD11	1.84	0.60
1:E:324:LEU:O	1:E:326:GLY:N	2.34	0.60
1:J:318:LYS:HZ2	1:J:328:THR:HG23	1.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:ARG:NH2	1:D:65:GLU:OE1	2.35	0.59
1:C:206:ASN:HB3	1:D:185:ARG:HG2	1.84	0.59
1:H:89:ILE:HG23	1:L:199:ILE:HD13	1.84	0.59
1:B:328:THR:H	1:B:453:SER:HA	1.66	0.59
1:C:344:LEU:HD11	1:C:427:LEU:HD13	1.82	0.59
1:F:380:ARG:HH21	1:F:422:PRO:HB2	1.67	0.59
1:E:213:LEU:O	1:E:217:ILE:HG13	2.03	0.59
1:E:222:GLU:O	1:E:225:VAL:HG22	2.03	0.59
1:L:368:GLN:H	1:L:380:ARG:HH12	1.50	0.59
1:D:53:LEU:HD11	1:D:62:LEU:HD13	1.84	0.59
1:G:351:LEU:HD21	1:G:378:PRO:HG2	1.84	0.59
1:I:440:ALA:HB3	1:I:475:ILE:HD12	1.84	0.59
1:C:221:SER:HB2	1:C:224:LYS:HB2	1.85	0.59
1:C:76:ILE:HD11	1:C:102:LEU:HD22	1.85	0.59
1:D:224:LYS:HE2	1:D:260:LEU:HD11	1.83	0.59
1:K:263:LYS:NZ	1:K:298:GLN:OE1	2.31	0.59
1:E:55:ASP:O	1:E:59:ILE:HG23	2.03	0.58
1:H:195:VAL:O	1:H:199:ILE:HG13	2.02	0.58
1:F:281:LEU:O	1:F:375:LYS:HE3	2.03	0.58
1:E:287:LEU:HD12	1:E:288:PRO:HD2	1.86	0.58
1:I:182:ASP:OD2	1:J:179:ARG:NH1	2.37	0.58
1:K:108:ARG:HG3	1:K:149:HIS:CE1	2.39	0.58
1:L:368:GLN:H	1:L:380:ARG:NH1	2.00	0.58
1:A:177:VAL:HB	1:A:205:VAL:HG22	1.86	0.58
1:D:225:VAL:HG21	1:D:257:ARG:HG3	1.84	0.58
1:J:316:ILE:O	1:J:320:MET:HG2	2.04	0.58
1:C:489:LYS:O	1:C:493:VAL:HG23	2.04	0.58
1:I:231:GLU:O	1:I:235:LEU:HD23	2.04	0.57
1:L:475:ILE:HG23	1:L:479:THR:HG21	1.86	0.57
1:B:284:LEU:O	1:B:375:LYS:NZ	2.30	0.57
1:E:42:GLY:O	1:E:44:ALA:N	2.29	0.57
1:G:351:LEU:HD11	1:G:370:LEU:HD22	1.85	0.57
1:L:59:ILE:HG21	1:L:88:TRP:HA	1.85	0.57
1:G:96:ARG:O	1:G:173:ARG:NH2	2.38	0.57
1:H:60:ARG:O	1:H:64:LEU:HB2	2.04	0.57
1:G:325:GLN:OE1	1:G:325:GLN:N	2.35	0.57
1:E:41:VAL:HB	1:E:160:ALA:HB2	1.86	0.57
1:J:27:GLU:OE2	1:J:31:ARG:NH2	2.35	0.57
1:I:337:HIS:HB3	1:I:344:LEU:HB3	1.87	0.57
1:G:90:ARG:HH21	1:I:174:ASN:HB3	1.70	0.57
1:I:286:GLN:HG2	1:I:376:ASP:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:OE2	1:A:31:ARG:NH2	2.38	0.57
1:E:37:LEU:HD12	1:E:47:LEU:CD1	2.34	0.57
1:J:250:GLU:OE1	1:J:253:ARG:NH1	2.38	0.57
1:K:401:ARG:NH1	1:K:492:GLU:OE2	2.37	0.57
1:K:421:LEU:HD23	1:K:425:ARG:HD3	1.86	0.57
1:G:104:THR:HG21	1:G:150:TRP:HB3	1.85	0.57
1:I:108:ARG:HG3	1:I:149:HIS:CE1	2.40	0.57
1:B:25:GLN:O	1:B:29:HIS:ND1	2.35	0.56
1:B:287:LEU:HD12	1:B:288:PRO:HD2	1.86	0.56
1:H:108:ARG:HH21	1:K:339:GLU:HA	1.69	0.56
1:H:200:GLN:NE2	1:H:468:ALA:O	2.38	0.56
1:I:287:LEU:HD12	1:I:288:PRO:HD2	1.88	0.56
1:I:401:ARG:HH21	1:I:492:GLU:HG2	1.70	0.56
1:B:327:GLY:O	1:B:328:THR:OG1	2.13	0.56
1:L:339:GLU:O	1:L:341:GLY:N	2.37	0.56
1:C:124:GLN:HB2	1:C:127:HIS:CE1	2.41	0.56
1:H:127:HIS:HA	1:H:130:ARG:HD2	1.87	0.56
1:I:318:LYS:HE3	1:I:328:THR:HB	1.85	0.56
1:I:340:LYS:HG2	1:K:108:ARG:HH22	1.70	0.56
1:A:276:THR:HG22	1:A:302:PHE:HE1	1.70	0.56
1:E:45:HIS:NE2	1:E:167:VAL:HG11	2.20	0.56
1:F:398:LEU:HD11	1:F:403:ARG:HG2	1.88	0.56
1:H:287:LEU:HD12	1:H:288:PRO:HD2	1.87	0.56
1:B:335:THR:HG22	1:B:346:LEU:HB3	1.87	0.56
1:J:61:ARG:HH11	1:J:64:LEU:HD23	1.69	0.56
1:L:42:GLY:O	1:L:44:ALA:N	2.33	0.56
1:C:10:PHE:HA	1:C:76:ILE:HG23	1.87	0.56
1:E:195:VAL:O	1:E:199:ILE:HG23	2.05	0.56
1:G:350:MET:HG3	1:G:351:LEU:HD12	1.87	0.56
1:J:214:VAL:HG22	1:J:284:LEU:HD22	1.86	0.56
1:C:282:HIS:NE2	1:D:212:ASP:OD1	2.38	0.56
1:F:331:MET:HG3	1:F:452:PHE:HB2	1.87	0.56
1:H:224:LYS:HE2	1:H:260:LEU:HD22	1.87	0.56
1:I:3:MET:O	1:I:5:ALA:N	2.35	0.56
1:C:212:ASP:OD1	1:D:282:HIS:NE2	2.37	0.56
1:D:95:LEU:HD13	1:D:97:LYS:H	1.70	0.56
1:J:287:LEU:HD12	1:J:288:PRO:HD2	1.88	0.56
1:B:7:GLU:HG2	1:B:46:VAL:CG2	2.36	0.56
1:J:380:ARG:HD2	1:J:422:PRO:O	2.06	0.56
1:H:275:THR:HG23	1:H:303:ALA:O	2.07	0.55
1:A:213:LEU:O	1:A:217:ILE:HG12	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:CYS:HB2	1:E:95:LEU:HB2	1.87	0.55
1:G:224:LYS:O	1:G:227:GLU:HG2	2.07	0.55
1:G:260:LEU:O	1:G:263:LYS:HG3	2.07	0.55
1:A:30:ALA:O	1:A:34:VAL:HG22	2.07	0.55
1:A:312:ALA:O	1:A:316:ILE:HG23	2.07	0.55
1:C:228:LEU:HD23	1:C:256:ALA:HB1	1.87	0.55
1:I:45:HIS:NE2	1:I:167:VAL:HG21	2.22	0.55
1:B:309:LYS:HZ2	1:B:402:PHE:HE1	1.55	0.55
1:F:417:ASP:OD1	1:F:418:MET:N	2.40	0.55
1:D:325:GLN:HB2	1:D:326:GLY:HA2	1.88	0.55
1:G:314:LEU:HD22	1:G:451:CYS:SG	2.46	0.55
1:J:409:VAL:HG12	1:J:430:PRO:HA	1.89	0.55
1:L:151:GLU:HA	1:L:156:ARG:NH1	2.21	0.55
1:B:195:VAL:O	1:B:199:ILE:HG13	2.06	0.55
1:I:339:GLU:O	1:I:341:GLY:N	2.34	0.55
1:L:240:PRO:HA	1:L:243:ARG:HH12	1.71	0.55
1:D:112:TRP:HH2	1:F:427:LEU:HD21	1.70	0.55
1:G:316:ILE:O	1:G:320:MET:HG2	2.07	0.55
1:L:64:LEU:HD13	1:L:94:ALA:HB1	1.89	0.55
1:A:475:ILE:HG23	1:A:479:THR:HG21	1.89	0.55
1:B:146:VAL:HG13	1:B:158:ARG:HD2	1.89	0.55
1:C:440:ALA:CB	1:C:475:ILE:HD12	2.36	0.55
1:I:437:SER:HA	1:I:475:ILE:HD11	1.88	0.55
1:B:151:GLU:HA	1:B:156:ARG:HH11	1.72	0.54
1:C:353:VAL:HG11	1:C:424:ALA:HB3	1.88	0.54
1:G:217:ILE:HD13	1:G:261:GLY:HA3	1.88	0.54
1:I:294:ARG:O	1:I:298:GLN:HG2	2.06	0.54
1:J:11:VAL:HG11	1:J:53:LEU:HD22	1.89	0.54
1:J:161:LYS:HD3	1:J:457:THR:HG21	1.89	0.54
1:B:29:HIS:HD2	1:B:106:PHE:CG	2.24	0.54
1:G:132:TYR:O	1:G:135:ILE:HG22	2.07	0.54
1:K:287:LEU:HD12	1:K:288:PRO:HD2	1.89	0.54
1:K:471:GLU:HG3	1:K:491:ASN:HD22	1.72	0.54
1:C:351:LEU:HD11	1:C:370:LEU:HD22	1.88	0.54
1:G:177:VAL:HB	1:G:205:VAL:HG22	1.89	0.54
1:D:316:ILE:O	1:D:320:MET:HG2	2.08	0.54
1:B:201:PHE:HZ	1:B:470:ILE:HD12	1.73	0.54
1:B:258:ILE:HD11	1:B:288:PRO:HG3	1.89	0.54
1:D:463:ASP:O	1:D:467:MET:HG3	2.07	0.54
1:E:161:LYS:O	1:E:165:THR:HG23	2.07	0.54
1:L:316:ILE:O	1:L:320:MET:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:SER:HB3	1:B:224:LYS:HD3	1.90	0.54
1:D:136:GLY:HA3	1:D:143:ARG:HD3	1.88	0.54
1:J:290:LEU:HD22	1:J:365:LEU:HD21	1.89	0.54
1:I:489:LYS:O	1:I:493:VAL:HG23	2.08	0.54
1:C:485:LYS:HG2	1:C:489:LYS:HE3	1.89	0.53
1:F:213:LEU:O	1:F:217:ILE:HG13	2.08	0.53
1:A:63:CYS:HB3	1:A:95:LEU:HB2	1.90	0.53
1:G:475:ILE:HG23	1:G:479:THR:HG21	1.90	0.53
1:I:282:HIS:NE2	1:J:212:ASP:OD1	2.40	0.53
1:J:255:GLN:HG3	1:J:379:ALA:HB3	1.89	0.53
1:G:19:GLY:C	1:G:21:GLU:H	2.11	0.53
1:G:287:LEU:HD12	1:G:288:PRO:HD2	1.91	0.53
1:I:76:ILE:HD12	1:I:159:LEU:HD21	1.91	0.53
1:D:253:ARG:O	1:D:257:ARG:HD3	2.08	0.53
1:D:317:MET:HE3	1:D:461:LEU:HD11	1.90	0.53
1:L:391:VAL:HG13	1:L:406:VAL:HG13	1.90	0.53
1:L:169:PHE:HE2	1:L:173:ARG:HH21	1.55	0.53
1:I:10:PHE:HA	1:I:76:ILE:HG23	1.89	0.53
1:K:59:ILE:HD11	1:K:87:MET:O	2.08	0.53
1:K:469:GLY:O	1:K:498:ARG:NH2	2.42	0.53
1:B:164:ARG:HD3	1:B:322:THR:HG22	1.90	0.53
1:K:195:VAL:O	1:K:199:ILE:HG23	2.08	0.53
1:F:301:GLY:HA2	1:F:314:LEU:CD1	2.39	0.53
1:A:287:LEU:HD12	1:A:288:PRO:HD2	1.91	0.53
1:D:380:ARG:HD2	1:D:422:PRO:O	2.08	0.53
1:E:132:TYR:O	1:E:135:ILE:HG22	2.09	0.53
1:K:96:ARG:O	1:K:173:ARG:NH2	2.35	0.53
1:L:213:LEU:O	1:L:217:ILE:HG13	2.09	0.53
1:D:229:LEU:HD22	1:D:253:ARG:HG2	1.90	0.52
1:G:191:GLU:HG2	1:H:194:LYS:HB2	1.89	0.52
1:L:240:PRO:HA	1:L:243:ARG:NH1	2.23	0.52
1:A:173:ARG:HB3	1:C:90:ARG:NH2	2.24	0.52
1:C:108:ARG:HG3	1:C:149:HIS:CE1	2.43	0.52
1:C:290:LEU:HD22	1:C:365:LEU:HD21	1.91	0.52
1:H:134:PHE:CG	1:K:189:VAL:HG12	2.44	0.52
1:H:400:HIS:CD2	1:H:496:ARG:HE	2.28	0.52
1:I:438:ALA:HB3	1:K:147:VAL:HG11	1.92	0.52
1:A:147:VAL:HG11	1:D:438:ALA:HB3	1.92	0.52
1:B:200:GLN:NE2	1:B:468:ALA:O	2.43	0.52
1:B:297:GLN:OE1	1:B:355:PRO:HG2	2.08	0.52
1:B:223:GLN:NE2	1:B:227:GLU:OE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:214:VAL:O	1:I:217:ILE:HG12	2.10	0.52
1:B:127:HIS:HA	1:B:130:ARG:HD2	1.92	0.52
1:C:328:THR:HG23	1:C:453:SER:HB2	1.90	0.52
1:C:433:SER:O	1:C:437:SER:HB2	2.10	0.52
1:G:162:TRP:HA	1:G:165:THR:HG22	1.92	0.52
1:H:255:GLN:NE2	1:H:286:GLN:OE1	2.42	0.52
1:A:438:ALA:HB3	1:F:147:VAL:HG11	1.92	0.52
1:B:344:LEU:HD13	1:B:427:LEU:HD23	1.91	0.52
1:C:89:ILE:HA	1:C:139:MET:HE1	1.91	0.52
1:J:327:GLY:HA3	1:J:356:SER:HB3	1.92	0.52
1:I:326:GLY:HA3	1:I:455:ALA:HB2	1.92	0.52
1:A:104:THR:HG22	1:A:105:GLN:H	1.74	0.52
1:F:86:LYS:O	1:F:89:ILE:HG12	2.10	0.52
1:F:224:LYS:HB3	1:F:260:LEU:HD13	1.92	0.52
1:J:7:GLU:HG2	1:J:71:VAL:HG12	1.92	0.52
1:F:407:ASN:ND2	1:F:475:ILE:O	2.40	0.52
1:G:179:ARG:HA	1:G:275:THR:HG22	1.92	0.52
1:H:63:CYS:HB2	1:H:95:LEU:HB2	1.90	0.52
1:B:161:LYS:HD3	1:B:164:ARG:HH21	1.75	0.51
1:B:213:LEU:O	1:B:217:ILE:HG13	2.10	0.51
1:B:309:LYS:HE3	1:B:397:ASP:HB2	1.91	0.51
1:I:45:HIS:CE1	1:I:167:VAL:HG21	2.45	0.51
1:A:104:THR:HG21	1:A:150:TRP:HB3	1.91	0.51
1:C:318:LYS:HE3	1:C:328:THR:HB	1.92	0.51
1:K:132:TYR:O	1:K:135:ILE:HG22	2.11	0.51
1:L:40:ALA:N	1:L:41:VAL:O	2.43	0.51
1:D:240:PRO:HA	1:D:243:ARG:NE	2.25	0.51
1:F:81:THR:HG22	1:F:122:LEU:O	2.10	0.51
1:G:442:ILE:HG23	1:L:133:GLY:HA3	1.91	0.51
1:H:151:GLU:HA	1:H:156:ARG:HH11	1.76	0.51
1:D:161:LYS:HZ1	1:D:457:THR:HG21	1.74	0.51
1:F:182:ASP:O	1:F:277:THR:HG21	2.10	0.51
1:F:391:VAL:HG13	1:F:406:VAL:HG13	1.92	0.51
1:I:339:GLU:C	1:I:341:GLY:H	2.13	0.51
1:K:299:GLY:O	1:K:315:ARG:NH1	2.43	0.51
1:C:132:TYR:O	1:C:135:ILE:HG22	2.11	0.51
1:C:214:VAL:O	1:C:217:ILE:HG12	2.09	0.51
1:F:475:ILE:HG23	1:F:479:THR:HG21	1.92	0.51
1:G:82:PHE:HB2	1:G:127:HIS:HE1	1.75	0.51
1:C:60:ARG:HD2	1:C:90:ARG:HD3	1.92	0.51
1:I:57:ASP:HA	1:I:60:ARG:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:LEU:HD21	1:C:378:PRO:HG2	1.91	0.51
1:A:335:THR:HG23	1:A:346:LEU:HB3	1.93	0.51
1:C:364:ILE:HB	1:C:382:VAL:HG23	1.93	0.51
1:H:348:SER:OG	1:H:349:HIS:N	2.43	0.51
1:H:435:ARG:NH2	1:I:152:ASP:OD2	2.44	0.51
1:I:433:SER:OG	1:I:436:ASP:OD1	2.24	0.51
1:K:179:ARG:NH2	1:L:182:ASP:OD2	2.44	0.51
1:L:34:VAL:HG21	1:L:49:TRP:HB2	1.93	0.51
1:L:331:MET:HB2	1:L:450:THR:O	2.10	0.51
1:A:217:ILE:HD13	1:A:261:GLY:HA3	1.92	0.51
1:A:244:GLN:O	1:A:249:ARG:HD2	2.11	0.51
1:B:103:HIS:CD2	1:E:442:ILE:HD11	2.46	0.51
1:F:240:PRO:HA	1:F:243:ARG:HD3	1.93	0.51
1:F:276:THR:HG22	1:F:302:PHE:CE1	2.46	0.51
1:H:53:LEU:HD12	1:H:59:ILE:HA	1.93	0.51
1:I:136:GLY:HA3	1:I:143:ARG:NH1	2.26	0.51
1:K:407:ASN:HD21	1:K:437:SER:HB2	1.76	0.51
1:L:364:ILE:HG22	1:L:382:VAL:HB	1.93	0.51
1:C:368:GLN:HB3	1:C:380:ARG:NH1	2.25	0.51
1:F:30:ALA:O	1:F:34:VAL:HG23	2.11	0.51
1:I:154:GLU:O	1:I:158:ARG:HG2	2.10	0.51
1:A:344:LEU:HD13	1:A:427:LEU:HD22	1.93	0.50
1:D:329:SER:OG	1:D:354:CYS:HB3	2.11	0.50
1:E:213:LEU:HD21	1:E:262:LEU:HD23	1.93	0.50
1:E:342:ASN:HB2	1:E:429:LYS:NZ	2.25	0.50
1:E:348:SER:OG	1:E:349:HIS:N	2.44	0.50
1:I:176:LYS:NZ	1:I:269:GLY:O	2.41	0.50
1:J:232:TYR:HE2	1:J:256:ALA:HB2	1.77	0.50
1:K:38:GLN:O	1:K:42:GLY:HA2	2.12	0.50
1:K:232:TYR:OH	1:K:259:GLU:OE1	2.23	0.50
1:E:177:VAL:HB	1:E:205:VAL:HG22	1.92	0.50
1:K:342:ASN:HB2	1:K:429:LYS:NZ	2.26	0.50
1:D:391:VAL:HG12	1:D:408:GLU:HG2	1.92	0.50
1:I:39:ALA:O	1:I:41:VAL:N	2.44	0.50
1:I:290:LEU:HD22	1:I:365:LEU:HD21	1.94	0.50
1:A:407:ASN:ND2	1:A:475:ILE:O	2.40	0.50
1:D:251:SER:HA	1:D:286:GLN:HE22	1.77	0.50
1:F:329:SER:OG	1:F:354:CYS:HB3	2.11	0.50
1:H:139:MET:HG2	1:L:199:ILE:HD12	1.94	0.50
1:I:296:MET:HE1	1:I:354:CYS:HB2	1.92	0.50
1:J:336:TYR:HD1	1:J:345:VAL:HG12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:328:THR:HG23	1:K:453:SER:HB2	1.92	0.50
1:H:96:ARG:O	1:H:173:ARG:NH2	2.36	0.50
1:H:103:HIS:CD2	1:K:442:ILE:HD11	2.46	0.50
1:J:189:VAL:CG2	1:J:396:ILE:HD11	2.41	0.50
1:E:326:GLY:HA2	1:E:455:ALA:HB2	1.93	0.50
1:G:38:GLN:O	1:G:42:GLY:N	2.43	0.50
1:H:10:PHE:HA	1:H:76:ILE:HG23	1.94	0.50
1:K:5:ALA:O	1:K:71:VAL:HG13	2.11	0.50
1:C:192:GLY:HA3	1:C:309:LYS:NZ	2.27	0.50
1:D:110:ILE:HD11	1:D:112:TRP:CH2	2.46	0.50
1:D:299:GLY:HA2	1:D:318:LYS:HD2	1.93	0.50
1:G:53:LEU:HD11	1:G:62:LEU:HG	1.93	0.50
1:G:360:GLU:HB3	1:G:361:GLU:C	2.31	0.50
1:H:85:ALA:HB1	1:H:135:ILE:HG13	1.93	0.50
1:H:89:ILE:O	1:H:93:LEU:HG	2.12	0.50
1:K:103:HIS:HB3	1:K:147:VAL:HG22	1.94	0.50
1:L:223:GLN:O	1:L:223:GLN:NE2	2.44	0.50
1:L:336:TYR:HD1	1:L:345:VAL:HG12	1.77	0.50
1:E:225:VAL:HG12	1:E:260:LEU:HD12	1.94	0.50
1:K:55:ASP:O	1:K:59:ILE:HG23	2.12	0.50
1:K:179:ARG:HD3	1:K:308:TRP:HB3	1.93	0.50
1:A:255:GLN:HG3	1:A:379:ALA:HB3	1.92	0.49
1:B:493:VAL:HG11	1:C:493:VAL:HG12	1.93	0.49
1:I:163:MET:O	1:I:167:VAL:HG23	2.12	0.49
1:J:85:ALA:HB2	1:J:131:GLU:HG3	1.94	0.49
1:L:177:VAL:HG22	1:L:273:ALA:HB3	1.93	0.49
1:B:124:GLN:HE21	1:E:334:TYR:HE1	1.60	0.49
1:D:16:HIS:CD2	1:D:54:LYS:HD2	2.47	0.49
1:G:312:ALA:O	1:G:316:ILE:HG23	2.12	0.49
1:J:175:LEU:HD11	1:J:315:ARG:HG2	1.94	0.49
1:L:200:GLN:NE2	1:L:468:ALA:O	2.44	0.49
1:B:255:GLN:HA	1:B:258:ILE:HG22	1.95	0.49
1:F:47:LEU:HD11	1:F:76:ILE:HD12	1.92	0.49
1:H:81:THR:OG1	1:H:82:PHE:N	2.45	0.49
1:J:323:GLY:HA2	1:J:324:LEU:HB2	1.95	0.49
1:K:116:ASP:OD1	1:K:117:MET:N	2.42	0.49
1:L:82:PHE:HB2	1:L:127:HIS:CE1	2.48	0.49
1:A:494:PHE:HD1	1:D:493:VAL:HG13	1.77	0.49
1:C:372:ILE:HD11	1:E:18:TYR:CE1	2.48	0.49
1:F:287:LEU:HD12	1:F:288:PRO:HD2	1.94	0.49
1:F:474:VAL:HG12	1:F:476:ASN:HD22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:485:LYS:O	1:I:489:LYS:HG3	2.13	0.49
1:I:493:VAL:HG11	1:K:493:VAL:HG13	1.95	0.49
1:K:348:SER:OG	1:K:349:HIS:N	2.45	0.49
1:B:9:TRP:CE2	1:B:50:LYS:HE3	2.47	0.49
1:B:228:LEU:HD11	1:B:294:ARG:HH21	1.78	0.49
1:C:96:ARG:O	1:C:173:ARG:NH2	2.45	0.49
1:D:127:HIS:HB2	1:F:448:HIS:HB2	1.95	0.49
1:F:268:ASP:OD1	1:F:269:GLY:N	2.46	0.49
1:H:276:THR:HG22	1:H:302:PHE:HE1	1.76	0.49
1:I:42:GLY:C	1:I:44:ALA:H	2.16	0.49
1:K:40:ALA:HB2	1:K:156:ARG:NH1	2.24	0.49
1:K:410:ASP:OD2	1:K:431:ARG:NH1	2.42	0.49
1:L:151:GLU:HA	1:L:156:ARG:HH12	1.77	0.49
1:L:177:VAL:HB	1:L:205:VAL:HG22	1.92	0.49
1:B:81:THR:OG1	1:B:124:GLN:OE1	2.30	0.49
1:C:33:MET:O	1:C:37:LEU:HD23	2.13	0.49
1:D:86:LYS:HA	1:D:89:ILE:HG13	1.94	0.49
1:K:81:THR:OG1	1:K:82:PHE:N	2.44	0.49
1:A:314:LEU:HD22	1:A:451:CYS:SG	2.52	0.49
1:C:403:ARG:NH1	1:C:444:ALA:O	2.45	0.49
1:D:457:THR:HG23	1:D:460:GLN:H	1.76	0.49
1:G:38:GLN:OE1	1:G:46:VAL:HA	2.13	0.49
1:H:400:HIS:HD2	1:H:496:ARG:HE	1.60	0.49
1:J:53:LEU:HD11	1:J:62:LEU:HD13	1.95	0.49
1:L:195:VAL:O	1:L:199:ILE:HG12	2.12	0.49
1:A:245:GLU:OE2	1:A:249:ARG:NH1	2.43	0.49
1:B:281:LEU:HD22	1:B:284:LEU:HD12	1.95	0.49
1:C:285:LYS:O	1:C:375:LYS:HB3	2.12	0.49
1:H:7:GLU:OE1	1:H:48:ARG:NH2	2.45	0.49
1:I:191:GLU:HG2	1:J:194:LYS:HB2	1.94	0.49
1:B:276:THR:HG22	1:B:302:PHE:HE1	1.77	0.49
1:C:186:GLU:O	1:E:86:LYS:HB2	2.13	0.49
1:E:82:PHE:H	1:E:124:GLN:HE21	1.61	0.49
1:E:297:GLN:HG3	1:E:355:PRO:HD2	1.94	0.49
1:G:366:ASP:OD2	1:G:368:GLN:NE2	2.46	0.49
1:A:34:VAL:CG2	1:A:35:PRO:HD3	2.40	0.49
1:H:221:SER:HB3	1:H:224:LYS:HB2	1.94	0.49
1:I:263:LYS:HG3	1:I:295:LEU:HD21	1.93	0.49
1:B:151:GLU:HA	1:B:156:ARG:NH1	2.28	0.48
1:C:480:SER:O	1:C:484:PHE:HB2	2.13	0.48
1:E:255:GLN:NE2	1:E:289:GLY:H	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:490:TRP:O	1:E:493:VAL:HG12	2.12	0.48
1:J:318:LYS:HZ1	1:J:328:THR:HG23	1.76	0.48
1:J:329:SER:OG	1:J:354:CYS:HB3	2.13	0.48
1:J:240:PRO:HA	1:J:243:ARG:NE	2.28	0.48
1:B:326:GLY:HA2	1:B:327:GLY:HA3	1.54	0.48
1:D:30:ALA:O	1:D:34:VAL:HG23	2.13	0.48
1:D:40:ALA:O	1:D:42:GLY:N	2.46	0.48
1:G:385:GLY:HA3	1:G:426:ILE:HG13	1.95	0.48
1:I:111:PRO:O	1:I:115:ILE:HG23	2.13	0.48
1:I:115:ILE:HG22	1:I:119:PHE:CD2	2.48	0.48
1:J:325:GLN:N	1:J:325:GLN:OE1	2.46	0.48
1:A:19:GLY:C	1:A:21:GLU:H	2.17	0.48
1:A:239:VAL:HG22	1:A:241:ALA:H	1.78	0.48
1:H:151:GLU:HA	1:H:156:ARG:NH1	2.28	0.48
1:I:168:ALA:HB1	1:I:316:ILE:HG23	1.95	0.48
1:B:201:PHE:CZ	1:B:470:ILE:HD12	2.48	0.48
1:G:421:LEU:HD23	1:G:425:ARG:HD2	1.93	0.48
1:K:190:THR:HG23	1:K:307:ASP:HA	1.94	0.48
1:A:332:GLU:HB2	1:A:349:HIS:HD2	1.79	0.48
1:A:493:VAL:HG23	1:F:494:PHE:HD1	1.79	0.48
1:B:134:PHE:CG	1:E:189:VAL:HG12	2.48	0.48
1:E:2:LYS:HD2	1:E:2:LYS:N	2.28	0.48
1:E:301:GLY:HA2	1:E:314:LEU:CD1	2.43	0.48
1:H:38:GLN:NE2	1:H:46:VAL:HA	2.28	0.48
1:C:421:LEU:HD13	1:C:425:ARG:HD3	1.95	0.48
1:F:385:GLY:HA3	1:F:426:ILE:HG13	1.95	0.48
1:F:276:THR:HG22	1:F:302:PHE:HE1	1.79	0.48
1:H:69:ASP:OD1	1:H:71:VAL:HG12	2.14	0.48
1:H:228:LEU:HD23	1:H:256:ALA:HB1	1.94	0.48
1:I:431:ARG:NH2	1:I:477:GLU:OE1	2.33	0.48
1:K:301:GLY:HA2	1:K:314:LEU:CD1	2.43	0.48
1:G:19:GLY:O	1:G:21:GLU:N	2.46	0.48
1:H:344:LEU:HD11	1:H:427:LEU:HB3	1.95	0.48
1:I:364:ILE:HB	1:I:382:VAL:HG22	1.95	0.48
1:J:149:HIS:CE1	1:J:151:GLU:HB2	2.49	0.48
1:L:50:LYS:HD2	1:L:62:LEU:HD11	1.96	0.48
1:A:405:ILE:HD12	1:A:444:ALA:HB3	1.95	0.48
1:B:228:LEU:HD22	1:B:260:LEU:HD21	1.96	0.48
1:C:177:VAL:HG22	1:C:273:ALA:HB3	1.95	0.48
1:D:339:GLU:O	1:D:341:GLY:N	2.47	0.48
1:E:9:TRP:HZ3	1:E:65:GLU:HG3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:440:ALA:HB3	1:I:475:ILE:CD1	2.44	0.48
1:J:457:THR:HG23	1:J:460:GLN:H	1.78	0.48
1:E:108:ARG:HG3	1:E:149:HIS:CE1	2.49	0.47
1:G:324:LEU:HB3	1:G:455:ALA:HB1	1.95	0.47
1:G:493:VAL:HG23	1:L:494:PHE:HD1	1.79	0.47
1:J:493:VAL:HG12	1:J:496:ARG:NH1	2.29	0.47
1:K:103:HIS:ND1	1:K:129:ASP:OD2	2.46	0.47
1:B:275:THR:HG23	1:B:303:ALA:O	2.14	0.47
1:E:471:GLU:HB2	1:E:495:TRP:CD1	2.48	0.47
1:J:391:VAL:HG12	1:J:408:GLU:HG2	1.97	0.47
1:K:12:VAL:HG23	1:K:52:VAL:HG23	1.97	0.47
1:A:493:VAL:HG22	1:A:496:ARG:NH1	2.29	0.47
1:G:328:THR:HG22	1:G:453:SER:OG	2.14	0.47
1:H:493:VAL:HG11	1:I:493:VAL:HG12	1.97	0.47
1:A:104:THR:HG23	1:A:148:GLY:O	2.14	0.47
1:A:282:HIS:NE2	1:B:212:ASP:OD1	2.47	0.47
1:C:188:ALA:HB2	1:E:86:LYS:HG3	1.96	0.47
1:C:194:LYS:HB2	1:D:191:GLU:HG2	1.96	0.47
1:A:40:ALA:CB	1:A:156:ARG:HE	2.28	0.47
1:A:93:LEU:HG	1:A:139:MET:HE1	1.97	0.47
1:K:12:VAL:HA	1:K:78:TRP:O	2.14	0.47
1:K:159:LEU:HD23	1:K:159:LEU:HA	1.74	0.47
1:A:179:ARG:NH2	1:A:183:ASN:OD1	2.48	0.47
1:G:387:GLU:OE1	1:G:413:LYS:HB2	2.14	0.47
1:H:276:THR:HG22	1:H:302:PHE:CE1	2.50	0.47
1:H:421:LEU:HD23	1:H:425:ARG:HD3	1.96	0.47
1:I:121:ASN:HA	1:I:124:GLN:NE2	2.28	0.47
1:L:239:VAL:O	1:L:241:ALA:N	2.47	0.47
1:L:339:GLU:OE1	1:L:342:ASN:ND2	2.44	0.47
1:C:135:ILE:HD12	1:C:135:ILE:HA	1.84	0.47
1:D:55:ASP:OD1	1:D:57:ASP:N	2.46	0.47
1:D:368:GLN:OE1	1:D:422:PRO:HG3	2.14	0.47
1:E:116:ASP:OD1	1:E:117:MET:N	2.45	0.47
1:F:318:LYS:HD2	1:F:328:THR:OG1	2.15	0.47
1:G:325:GLN:HA	1:G:326:GLY:HA3	1.65	0.47
1:J:233:GLU:OE2	1:J:249:ARG:NH2	2.41	0.47
1:L:53:LEU:HD13	1:L:59:ILE:HD13	1.95	0.47
1:D:239:VAL:HG22	1:D:241:ALA:H	1.80	0.47
1:G:154:GLU:HA	1:G:157:GLU:HG2	1.96	0.47
1:I:348:SER:OG	1:I:349:HIS:N	2.46	0.47
1:A:385:GLY:HA3	1:A:426:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:ARG:HD3	1:J:441:TRP:CD1	2.50	0.47
1:A:334:TYR:HE2	1:A:349:HIS:HA	1.80	0.47
1:B:107:ASN:ND2	1:B:109:ASP:O	2.48	0.47
1:F:348:SER:HB2	1:F:424:ALA:O	2.15	0.47
1:G:7:GLU:HG2	1:G:71:VAL:HG12	1.97	0.47
1:G:104:THR:HG22	1:G:105:GLN:N	2.30	0.47
1:G:309:LYS:HD2	1:G:395:LEU:HD12	1.95	0.47
1:I:50:LYS:HG3	1:I:62:LEU:HD11	1.97	0.47
1:I:53:LEU:HD11	1:I:62:LEU:HG	1.96	0.47
1:B:10:PHE:HA	1:B:76:ILE:HG23	1.96	0.46
1:B:471:GLU:HB2	1:B:495:TRP:CD1	2.50	0.46
1:C:195:VAL:O	1:C:199:ILE:HG13	2.16	0.46
1:E:362:LYS:N	1:E:362:LYS:HD2	2.30	0.46
1:G:355:PRO:HA	1:G:383:PHE:CZ	2.50	0.46
1:H:224:LYS:HE2	1:H:224:LYS:HB3	1.67	0.46
1:I:86:LYS:HA	1:I:89:ILE:HG13	1.97	0.46
1:J:34:VAL:HB	1:J:35:PRO:HD3	1.97	0.46
1:J:67:SER:HB3	1:J:96:ARG:H	1.80	0.46
1:K:85:ALA:HB1	1:K:135:ILE:HB	1.97	0.46
1:D:342:ASN:HA	1:D:429:LYS:HE3	1.97	0.46
1:E:146:VAL:HG12	1:E:158:ARG:HE	1.80	0.46
1:E:323:GLY:O	1:E:325:GLN:N	2.48	0.46
1:I:89:ILE:HA	1:I:139:MET:HE1	1.97	0.46
1:I:407:ASN:HA	1:I:475:ILE:HG23	1.97	0.46
1:F:214:VAL:HG21	1:F:283:GLY:HA3	1.97	0.46
1:G:334:TYR:HE2	1:G:349:HIS:HA	1.80	0.46
1:H:471:GLU:HB2	1:H:495:TRP:CD1	2.51	0.46
1:L:474:VAL:HG12	1:L:476:ASN:HD22	1.81	0.46
1:B:90:ARG:NH2	1:F:202:GLY:O	2.49	0.46
1:G:82:PHE:HB2	1:G:127:HIS:CE1	2.51	0.46
1:G:151:GLU:HA	1:G:156:ARG:NH1	2.31	0.46
1:G:269:GLY:HA3	1:G:271:PHE:CE2	2.51	0.46
1:L:301:GLY:HA2	1:L:314:LEU:CD1	2.45	0.46
1:A:29:HIS:O	1:A:33:MET:HG3	2.15	0.46
1:C:334:TYR:HE2	1:C:349:HIS:HA	1.81	0.46
1:F:54:LYS:H	1:F:54:LYS:HG2	1.65	0.46
1:F:376:ASP:OD1	1:F:377:ASP:N	2.48	0.46
1:I:269:GLY:HA3	1:I:271:PHE:CE2	2.50	0.46
1:K:95:LEU:HD23	1:K:99:LEU:HD21	1.97	0.46
1:B:323:GLY:HA2	1:B:324:LEU:HA	1.76	0.46
1:C:121:ASN:HA	1:C:124:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:LYS:O	1:D:165:THR:HG22	2.16	0.46
1:E:471:GLU:HG3	1:E:491:ASN:HD22	1.80	0.46
1:F:490:TRP:O	1:F:493:VAL:HG12	2.16	0.46
1:J:85:ALA:HB1	1:J:135:ILE:HB	1.97	0.46
1:J:134:PHE:CG	1:L:189:VAL:HG22	2.49	0.46
1:A:132:TYR:O	1:A:135:ILE:HG22	2.16	0.46
1:C:203:TRP:HH2	1:C:395:LEU:HD22	1.80	0.46
1:E:384:ASP:CG	1:E:414:PRO:HG3	2.36	0.46
1:G:421:LEU:HD11	1:L:120:MET:SD	2.56	0.46
1:E:220:VAL:HG11	1:E:257:ARG:HG3	1.98	0.46
1:E:343:ASP:HB3	1:E:434:LEU:HD22	1.98	0.46
1:F:195:VAL:O	1:F:199:ILE:HG12	2.16	0.46
1:F:301:GLY:HA2	1:F:314:LEU:HD11	1.97	0.46
1:G:126:ALA:O	1:G:130:ARG:HG3	2.16	0.46
1:G:401:ARG:HH21	1:G:492:GLU:HG2	1.81	0.46
1:I:228:LEU:HD23	1:I:256:ALA:HB1	1.98	0.46
1:J:86:LYS:HG3	1:L:188:ALA:HB2	1.96	0.46
1:K:26:VAL:HG22	1:K:80:HIS:CD2	2.51	0.46
1:L:45:HIS:CD2	1:L:167:VAL:HG21	2.51	0.46
1:L:168:ALA:HB2	1:L:320:MET:HB3	1.98	0.46
1:D:183:ASN:HD22	1:D:190:THR:HG23	1.81	0.46
1:E:53:LEU:HD11	1:E:62:LEU:HG	1.98	0.46
1:G:76:ILE:HG23	1:G:100:LEU:HD12	1.98	0.46
1:K:149:HIS:CE1	1:K:151:GLU:HB2	2.51	0.46
1:K:211:GLY:O	1:K:215:GLN:NE2	2.49	0.46
1:A:351:LEU:HD21	1:A:378:PRO:HG2	1.98	0.46
1:C:317:MET:HA	1:C:320:MET:HG2	1.98	0.46
1:H:463:ASP:O	1:H:467:MET:HG3	2.15	0.46
1:I:124:GLN:HB2	1:I:127:HIS:NE2	2.30	0.46
1:C:431:ARG:HE	1:C:477:GLU:HG3	1.80	0.45
1:G:64:LEU:HD23	1:G:64:LEU:HA	1.86	0.45
1:J:368:GLN:O	1:J:380:ARG:NH2	2.50	0.45
1:L:418:MET:O	1:L:425:ARG:NH2	2.49	0.45
1:C:38:GLN:NE2	1:C:45:HIS:O	2.44	0.45
1:C:287:LEU:HD12	1:C:288:PRO:HD2	1.96	0.45
1:D:67:SER:HB3	1:D:96:ARG:H	1.81	0.45
1:F:281:LEU:HD22	1:F:284:LEU:HD12	1.97	0.45
1:H:164:ARG:HD2	1:H:322:THR:HG22	1.99	0.45
1:K:37:LEU:HD13	1:K:37:LEU:O	2.16	0.45
1:A:38:GLN:HE22	1:A:46:VAL:HA	1.80	0.45
1:A:171:GLU:HG3	1:A:319:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LYS:HG3	1:A:295:LEU:HD11	1.98	0.45
1:D:34:VAL:HB	1:D:35:PRO:HD3	1.98	0.45
1:D:175:LEU:HD11	1:D:315:ARG:HG2	1.99	0.45
1:E:14:SER:OG	1:E:15:GLN:N	2.49	0.45
1:G:213:LEU:O	1:G:217:ILE:HG12	2.16	0.45
1:H:12:VAL:HA	1:H:78:TRP:O	2.16	0.45
1:H:16:HIS:CE1	1:H:54:LYS:HD3	2.51	0.45
1:K:463:ASP:O	1:K:467:MET:HG3	2.17	0.45
1:K:490:TRP:O	1:K:493:VAL:HG12	2.15	0.45
1:C:11:VAL:HG22	1:C:50:LYS:HB3	1.97	0.45
1:C:312:ALA:O	1:C:316:ILE:HG22	2.17	0.45
1:D:233:GLU:OE2	1:D:249:ARG:NH2	2.47	0.45
1:E:85:ALA:HB1	1:E:135:ILE:HB	1.99	0.45
1:F:263:LYS:CE	1:F:298:GLN:HE22	2.28	0.45
1:I:319:VAL:O	1:I:322:THR:HG23	2.17	0.45
1:A:53:LEU:HD11	1:A:62:LEU:HG	1.98	0.45
1:A:86:LYS:HG3	1:D:188:ALA:HB2	1.97	0.45
1:A:315:ARG:O	1:A:319:VAL:HG12	2.17	0.45
1:E:178:ALA:O	1:E:274:PHE:HA	2.15	0.45
1:L:81:THR:HG22	1:L:122:LEU:O	2.17	0.45
1:L:463:ASP:O	1:L:467:MET:HG3	2.16	0.45
1:C:314:LEU:HD12	1:C:330:PHE:HB2	1.99	0.45
1:E:81:THR:OG1	1:E:82:PHE:N	2.50	0.45
1:F:64:LEU:HD13	1:F:94:ALA:HB1	1.98	0.45
1:F:316:ILE:O	1:F:320:MET:HG2	2.17	0.45
1:J:269:GLY:HA3	1:J:271:PHE:CE1	2.51	0.45
1:A:425:ARG:HD3	1:A:425:ARG:N	2.32	0.45
1:D:11:VAL:HG11	1:D:53:LEU:HD22	1.99	0.45
1:D:291:ALA:O	1:D:295:LEU:HG	2.16	0.45
1:L:12:VAL:HA	1:L:78:TRP:O	2.17	0.45
1:C:192:GLY:HA3	1:C:309:LYS:HZ1	1.82	0.45
1:D:336:TYR:CE1	1:D:434:LEU:HD21	2.52	0.45
1:E:321:SER:HB2	1:E:455:ALA:HB3	1.99	0.45
1:F:360:GLU:H	1:F:360:GLU:CD	2.19	0.45
1:I:85:ALA:HB2	1:I:131:GLU:HG3	1.99	0.45
1:I:335:THR:HG23	1:K:105:GLN:OE1	2.17	0.45
1:A:151:GLU:HA	1:A:156:ARG:NH1	2.32	0.45
1:A:485:LYS:HD2	1:A:485:LYS:HA	1.75	0.45
1:C:7:GLU:HA	1:C:46:VAL:HG13	1.98	0.45
1:C:463:ASP:O	1:C:467:MET:HG3	2.17	0.45
1:E:12:VAL:HA	1:E:78:TRP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:53:LEU:HD13	1:H:62:LEU:HD23	1.99	0.45
1:H:64:LEU:HD21	1:L:67:SER:O	2.16	0.45
1:H:344:LEU:HD13	1:H:345:VAL:N	2.32	0.45
1:I:132:TYR:O	1:I:135:ILE:HG22	2.17	0.45
1:K:163:MET:O	1:K:167:VAL:HG13	2.17	0.45
1:L:274:PHE:O	1:L:302:PHE:HA	2.17	0.45
1:L:281:LEU:O	1:L:375:LYS:HE3	2.17	0.45
1:A:86:LYS:HE3	1:D:186:GLU:HA	1.99	0.45
1:D:259:GLU:HG3	1:D:295:LEU:HD21	1.98	0.45
1:G:304:GLY:O	1:G:305:GLU:HG2	2.17	0.45
1:H:20:ASP:O	1:H:23:LEU:HB2	2.17	0.45
1:H:149:HIS:ND1	1:H:151:GLU:HB2	2.32	0.45
1:J:463:ASP:O	1:J:467:MET:HG3	2.16	0.45
1:L:312:ALA:O	1:L:316:ILE:HG23	2.16	0.45
1:A:162:TRP:HA	1:A:165:THR:HG22	1.99	0.44
1:B:53:LEU:H	1:B:53:LEU:HD23	1.82	0.44
1:D:90:ARG:HH21	1:E:204:SER:HB3	1.80	0.44
1:D:368:GLN:HG2	1:D:369:HIS:H	1.82	0.44
1:H:475:ILE:HG23	1:H:479:THR:HG21	1.99	0.44
1:I:11:VAL:HG22	1:I:50:LYS:HB3	2.00	0.44
1:J:86:LYS:HB2	1:L:186:GLU:O	2.17	0.44
1:L:224:LYS:HB3	1:L:260:LEU:HD13	2.00	0.44
1:L:301:GLY:HA2	1:L:314:LEU:HD11	2.00	0.44
1:L:351:LEU:HD11	1:L:378:PRO:HG2	1.98	0.44
1:C:438:ALA:HB3	1:E:147:VAL:HG11	1.99	0.44
1:I:285:LYS:O	1:I:375:LYS:HB3	2.17	0.44
1:K:7:GLU:HG3	1:K:71:VAL:HG12	1.99	0.44
1:L:217:ILE:HD12	1:L:284:LEU:HD21	1.98	0.44
1:L:221:SER:HB2	1:L:224:LYS:HE3	2.00	0.44
1:L:333:ASP:OD1	1:L:333:ASP:N	2.50	0.44
1:A:222:GLU:C	1:A:224:LYS:H	2.20	0.44
1:C:296:MET:HE3	1:C:314:LEU:HD11	1.99	0.44
1:D:53:LEU:HB3	1:D:59:ILE:HG12	2.00	0.44
1:E:96:ARG:HB2	1:E:173:ARG:HH22	1.81	0.44
1:E:159:LEU:HD23	1:E:159:LEU:HA	1.75	0.44
1:G:224:LYS:HB3	1:G:224:LYS:HE2	1.86	0.44
1:K:59:ILE:HD11	1:K:87:MET:C	2.38	0.44
1:K:292:VAL:HG21	1:K:352:GLU:HB3	1.99	0.44
1:A:348:SER:HB2	1:A:424:ALA:O	2.17	0.44
1:B:465:ALA:HA	1:B:470:ILE:HG22	2.00	0.44
1:H:438:ALA:HB3	1:I:147:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:228:LEU:HD11	1:I:294:ARG:HH21	1.81	0.44
1:J:97:LYS:HD3	1:J:173:ARG:HH22	1.82	0.44
1:L:277:THR:HG22	1:L:305:GLU:HA	1.99	0.44
1:L:368:GLN:N	1:L:380:ARG:NH1	2.64	0.44
1:D:392:ASN:HA	1:D:451:CYS:O	2.18	0.44
1:H:186:GLU:O	1:I:86:LYS:HB2	2.17	0.44
1:L:321:SER:O	1:L:321:SER:OG	2.32	0.44
1:A:190:THR:HG23	1:A:307:ASP:HA	1.99	0.44
1:A:229:LEU:HD21	1:A:253:ARG:HA	1.99	0.44
1:B:89:ILE:HG23	1:F:199:ILE:HD13	1.98	0.44
1:D:55:ASP:OD2	1:D:58:GLU:HG3	2.17	0.44
1:E:351:LEU:HD21	1:E:370:LEU:HD22	1.99	0.44
1:G:438:ALA:HB3	1:L:147:VAL:HG11	1.99	0.44
1:K:14:SER:HB2	1:K:81:THR:CG2	2.48	0.44
1:A:7:GLU:HG2	1:A:71:VAL:HG12	2.00	0.44
1:B:41:VAL:HG13	1:B:160:ALA:CB	2.42	0.44
1:B:213:LEU:HD22	1:B:217:ILE:HD11	2.00	0.44
1:B:337:HIS:O	1:B:343:ASP:HA	2.17	0.44
1:L:149:HIS:CE1	1:L:151:GLU:HB2	2.52	0.44
1:L:398:LEU:HD11	1:L:403:ARG:HG2	1.98	0.44
1:B:276:THR:HG22	1:B:302:PHE:CE1	2.52	0.44
1:B:336:TYR:HD1	1:B:345:VAL:HG22	1.83	0.44
1:C:239:VAL:HG22	1:C:241:ALA:H	1.83	0.44
1:G:222:GLU:OE2	1:G:257:ARG:NH1	2.51	0.44
1:G:403:ARG:NH1	1:G:444:ALA:O	2.45	0.44
1:H:53:LEU:HD23	1:H:53:LEU:H	1.83	0.44
1:H:183:ASN:ND2	1:H:190:THR:HG22	2.33	0.44
1:I:405:ILE:HD12	1:I:446:GLY:HA2	1.99	0.44
1:K:53:LEU:HD13	1:K:59:ILE:HA	1.99	0.44
1:A:304:GLY:O	1:A:305:GLU:HG2	2.18	0.44
1:B:86:LYS:HA	1:B:89:ILE:HG13	2.00	0.44
1:B:336:TYR:CD1	1:B:345:VAL:HG22	2.52	0.44
1:C:471:GLU:HB2	1:C:495:TRP:CD1	2.52	0.44
1:G:229:LEU:HD21	1:G:253:ARG:HA	2.00	0.44
1:G:293:GLN:HE21	1:G:353:VAL:H	1.66	0.44
1:G:411:ALA:HA	1:G:428:TRP:HA	2.00	0.44
1:I:27:GLU:OE2	1:I:31:ARG:NH2	2.51	0.44
1:L:276:THR:HG22	1:L:302:PHE:CE1	2.53	0.44
1:A:222:GLU:O	1:A:224:LYS:N	2.44	0.43
1:D:135:ILE:HD12	1:D:135:ILE:HA	1.92	0.43
1:G:333:ASP:OD1	1:G:333:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:ALA:HB2	1:L:96:ARG:NH2	2.33	0.43
1:I:188:ALA:HB2	1:K:86:LYS:HG3	1.99	0.43
1:J:132:TYR:O	1:J:135:ILE:HG22	2.16	0.43
1:K:405:ILE:HA	1:K:473:VAL:HG23	2.00	0.43
1:E:312:ALA:O	1:E:316:ILE:HG13	2.18	0.43
1:F:200:GLN:NE2	1:F:468:ALA:O	2.50	0.43
1:J:314:LEU:O	1:J:318:LYS:HB2	2.18	0.43
1:L:225:VAL:HG21	1:L:257:ARG:HG2	2.00	0.43
1:B:2:LYS:HD2	1:B:2:LYS:HA	1.82	0.43
1:B:204:SER:HB2	1:F:90:ARG:HH22	1.83	0.43
1:C:60:ARG:HA	1:C:63:CYS:SG	2.59	0.43
1:C:243:ARG:HG2	1:C:243:ARG:HH11	1.82	0.43
1:D:159:LEU:HD23	1:D:159:LEU:HA	1.87	0.43
1:D:335:THR:HG23	1:D:346:LEU:HB3	2.00	0.43
1:F:336:TYR:HD1	1:F:345:VAL:HG12	1.81	0.43
1:I:195:VAL:O	1:I:199:ILE:HG13	2.19	0.43
1:B:430:PRO:HG2	1:B:434:LEU:HA	2.00	0.43
1:E:299:GLY:O	1:E:315:ARG:NH1	2.51	0.43
1:I:16:HIS:CE1	1:I:54:LYS:HB2	2.53	0.43
1:I:244:GLN:HG3	1:I:245:GLU:H	1.83	0.43
1:D:364:ILE:HG13	1:D:382:VAL:HB	2.00	0.43
1:D:368:GLN:HG2	1:D:369:HIS:N	2.34	0.43
1:F:263:LYS:HE2	1:F:298:GLN:HE22	1.82	0.43
1:G:348:SER:HB2	1:G:424:ALA:O	2.18	0.43
1:L:120:MET:O	1:L:124:GLN:HG3	2.19	0.43
1:C:489:LYS:HG2	1:E:494:PHE:CZ	2.54	0.43
1:K:184:MET:HB3	1:K:187:VAL:HG21	2.00	0.43
1:K:282:HIS:NE2	1:L:212:ASP:OD1	2.50	0.43
1:L:339:GLU:C	1:L:341:GLY:H	2.20	0.43
1:A:304:GLY:C	1:A:305:GLU:HG2	2.39	0.43
1:A:489:LYS:HD2	1:F:494:PHE:CE2	2.54	0.43
1:D:149:HIS:CE1	1:D:151:GLU:HB2	2.54	0.43
1:D:345:VAL:O	1:D:427:LEU:HA	2.19	0.43
1:F:239:VAL:HG23	1:F:365:LEU:O	2.19	0.43
1:G:349:HIS:O	1:G:423:VAL:HG21	2.19	0.43
1:I:124:GLN:HB2	1:I:127:HIS:CD2	2.54	0.43
1:L:418:MET:CB	1:L:425:ARG:HH21	2.30	0.43
1:B:438:ALA:HB3	1:C:147:VAL:HG11	2.01	0.43
1:F:303:ALA:HB3	1:F:307:ASP:O	2.18	0.43
1:G:334:TYR:HE1	1:L:124:GLN:HE21	1.67	0.43
1:G:359:ALA:HB3	1:G:386:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:ALA:HB2	1:H:156:ARG:HE	1.83	0.43
1:H:217:ILE:O	1:H:220:VAL:HG22	2.19	0.43
1:I:326:GLY:CA	1:I:455:ALA:HB2	2.49	0.43
1:L:348:SER:HB2	1:L:424:ALA:O	2.19	0.43
1:C:63:CYS:HB2	1:C:95:LEU:HB2	1.99	0.43
1:D:143:ARG:HE	1:D:143:ARG:HB2	1.49	0.43
1:E:301:GLY:HA2	1:E:314:LEU:HD11	2.01	0.43
1:E:413:LYS:HD2	1:E:413:LYS:HA	1.74	0.43
1:H:5:ALA:O	1:H:71:VAL:HG23	2.19	0.43
1:H:16:HIS:HE1	1:H:54:LYS:HD3	1.82	0.43
1:J:135:ILE:HD12	1:J:135:ILE:HA	1.88	0.43
1:A:126:ALA:O	1:A:130:ARG:HG3	2.19	0.43
1:E:40:ALA:HB2	1:E:156:ARG:NH1	2.31	0.43
1:F:286:GLN:HE21	1:F:378:PRO:CA	2.16	0.43
1:L:45:HIS:NE2	1:L:167:VAL:HG21	2.34	0.43
1:L:286:GLN:HB3	1:L:378:PRO:HB3	2.00	0.43
1:A:26:VAL:HG22	1:A:80:HIS:CD2	2.54	0.42
1:A:186:GLU:HA	1:F:86:LYS:HD2	2.00	0.42
1:E:5:ALA:O	1:E:71:VAL:HG13	2.19	0.42
1:E:290:LEU:HD23	1:E:294:ARG:HG3	2.00	0.42
1:G:250:GLU:OE2	1:G:253:ARG:NH1	2.52	0.42
1:G:302:PHE:HE2	1:G:352:GLU:HG3	1.83	0.42
1:G:401:ARG:NH2	1:G:492:GLU:HA	2.34	0.42
1:K:404:LEU:HD21	1:K:461:LEU:HD22	2.01	0.42
1:B:465:ALA:CB	1:B:472:CYS:HB2	2.49	0.42
1:C:50:LYS:HD2	1:C:50:LYS:HA	1.70	0.42
1:D:289:GLY:O	1:D:293:GLN:HG2	2.18	0.42
1:I:135:ILE:HD12	1:I:135:ILE:HA	1.86	0.42
1:J:133:GLY:HA2	1:J:143:ARG:HH12	1.84	0.42
1:K:301:GLY:HA2	1:K:314:LEU:HD12	2.01	0.42
1:L:132:TYR:O	1:L:135:ILE:HG22	2.19	0.42
1:B:342:ASN:HA	1:B:429:LYS:NZ	2.34	0.42
1:C:171:GLU:OE1	1:C:315:ARG:NH1	2.52	0.42
1:C:296:MET:HE1	1:C:354:CYS:HB2	2.01	0.42
1:D:336:TYR:HD1	1:D:345:VAL:HG12	1.85	0.42
1:F:274:PHE:O	1:F:302:PHE:HA	2.19	0.42
1:G:1:MET:N	1:G:298:GLN:HG3	2.34	0.42
1:I:29:HIS:O	1:I:33:MET:HG3	2.18	0.42
1:I:177:VAL:HB	1:I:205:VAL:HG22	2.02	0.42
1:K:42:GLY:C	1:K:44:ALA:H	2.18	0.42
1:A:195:VAL:HG13	1:C:89:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:MET:C	1:A:351:LEU:HD12	2.39	0.42
1:C:111:PRO:O	1:C:115:ILE:HG23	2.19	0.42
1:C:431:ARG:O	1:C:437:SER:OG	2.36	0.42
1:G:304:GLY:C	1:G:305:GLU:HG2	2.39	0.42
1:G:360:GLU:HA	1:G:361:GLU:HB3	2.00	0.42
1:H:159:LEU:HD23	1:H:159:LEU:HA	1.86	0.42
1:I:63:CYS:HB2	1:I:95:LEU:HB2	2.00	0.42
1:I:330:PHE:CZ	1:I:449:HIS:CD2	3.07	0.42
1:J:115:ILE:HG13	1:J:119:PHE:HD2	1.84	0.42
1:L:7:GLU:HG2	1:L:71:VAL:HG12	2.02	0.42
1:B:245:GLU:OE2	1:B:245:GLU:N	2.53	0.42
1:B:475:ILE:HG23	1:B:479:THR:HG21	2.01	0.42
1:E:38:GLN:O	1:E:42:GLY:HA2	2.19	0.42
1:E:59:ILE:HD11	1:E:87:MET:O	2.19	0.42
1:E:191:GLU:HG2	1:F:194:LYS:HB2	2.01	0.42
1:F:132:TYR:O	1:F:135:ILE:HG22	2.20	0.42
1:H:44:ALA:HA	1:H:45:HIS:HA	1.75	0.42
1:H:213:LEU:HD22	1:H:217:ILE:HD11	2.01	0.42
1:J:90:ARG:HH21	1:K:204:SER:HB3	1.84	0.42
1:J:348:SER:HB2	1:J:424:ALA:O	2.20	0.42
1:A:303:ALA:HB3	1:A:307:ASP:O	2.20	0.42
1:A:405:ILE:HD11	1:A:475:ILE:HD11	2.01	0.42
1:B:55:ASP:HB3	1:B:58:GLU:OE2	2.19	0.42
1:B:186:GLU:O	1:C:86:LYS:HB2	2.18	0.42
1:B:240:PRO:HA	1:B:243:ARG:HG2	2.01	0.42
1:C:14:SER:OG	1:C:81:THR:HG22	2.20	0.42
1:C:250:GLU:HA	1:C:253:ARG:HG2	2.01	0.42
1:G:183:ASN:ND2	1:G:190:THR:HG22	2.34	0.42
1:G:303:ALA:HB3	1:G:307:ASP:O	2.19	0.42
1:H:158:ARG:NH1	1:H:459:GLU:OE1	2.53	0.42
1:H:274:PHE:CZ	1:H:292:VAL:HG22	2.55	0.42
1:J:494:PHE:CE2	1:L:489:LYS:HD3	2.54	0.42
1:L:263:LYS:HE2	1:L:298:GLN:HE22	1.84	0.42
1:D:147:VAL:HG11	1:F:438:ALA:HB3	2.00	0.42
1:E:59:ILE:CD1	1:E:88:TRP:HA	2.46	0.42
1:F:403:ARG:NH1	1:F:444:ALA:O	2.52	0.42
1:I:232:TYR:OH	1:I:259:GLU:OE1	2.31	0.42
1:I:314:LEU:HA	1:I:451:CYS:SG	2.60	0.42
1:K:177:VAL:HB	1:K:205:VAL:HG22	2.01	0.42
1:A:154:GLU:O	1:A:157:GLU:HG2	2.20	0.42
1:B:228:LEU:HD21	1:B:259:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:THR:HG22	1:E:148:GLY:O	2.20	0.42
1:E:343:ASP:OD2	1:E:435:ARG:NH1	2.52	0.42
1:I:289:GLY:CA	1:I:351:LEU:HD13	2.50	0.42
1:J:361:GLU:H	1:J:361:GLU:HG3	1.66	0.42
1:C:144:LYS:NZ	1:C:459:GLU:OE2	2.42	0.42
1:D:177:VAL:HB	1:D:205:VAL:HG22	2.01	0.42
1:E:53:LEU:HD13	1:E:59:ILE:HA	2.02	0.42
1:E:485:LYS:HE3	1:E:485:LYS:HB3	1.79	0.42
1:J:146:VAL:HG13	1:J:158:ARG:HD2	2.00	0.42
1:J:147:VAL:HB	1:L:435:ARG:HG2	2.01	0.42
1:L:31:ARG:HH12	1:L:49:TRP:HE1	1.67	0.42
1:A:6:TYR:HA	1:A:71:VAL:O	2.20	0.42
1:A:44:ALA:HA	1:A:45:HIS:HA	1.79	0.42
1:A:104:THR:HG22	1:A:105:GLN:N	2.35	0.42
1:D:23:LEU:HD21	1:D:54:LYS:HD3	2.01	0.42
1:E:331:MET:HG3	1:E:452:PHE:HB2	2.01	0.42
1:F:53:LEU:HD13	1:F:59:ILE:CD1	2.46	0.42
1:F:108:ARG:HG3	1:F:149:HIS:CD2	2.55	0.42
1:G:316:ILE:HA	1:G:319:VAL:HG12	2.01	0.42
1:H:134:PHE:CD1	1:K:189:VAL:HG12	2.55	0.42
1:J:342:ASN:OD1	1:J:429:LYS:NZ	2.34	0.42
1:J:377:ASP:HA	1:J:378:PRO:HD3	1.90	0.42
1:K:318:LYS:HD2	1:K:328:THR:HB	2.02	0.42
1:L:182:ASP:O	1:L:277:THR:HG21	2.20	0.42
1:A:225:VAL:HG21	1:A:257:ARG:HG2	2.02	0.41
1:B:255:GLN:CG	1:B:290:LEU:HB3	2.44	0.41
1:F:135:ILE:HD12	1:F:135:ILE:HA	1.84	0.41
1:F:471:GLU:HB2	1:F:495:TRP:CD1	2.55	0.41
1:H:213:LEU:HD11	1:H:262:LEU:HD21	2.02	0.41
1:I:50:LYS:HD2	1:I:50:LYS:HA	1.80	0.41
1:J:281:LEU:HD11	1:J:287:LEU:HD13	2.00	0.41
1:A:124:GLN:HB3	1:A:127:HIS:CE1	2.54	0.41
1:A:299:GLY:O	1:A:315:ARG:NH1	2.53	0.41
1:A:322:THR:O	1:A:322:THR:HG22	2.19	0.41
1:E:16:HIS:CE1	1:E:54:LYS:HD2	2.55	0.41
1:E:391:VAL:HG22	1:E:408:GLU:HG2	2.01	0.41
1:G:401:ARG:NH1	1:G:471:GLU:OE1	2.49	0.41
1:I:255:GLN:HB3	1:I:290:LEU:HB3	2.02	0.41
1:K:280:ASP:OD1	1:L:209:GLY:HA3	2.20	0.41
1:L:450:THR:O	1:L:450:THR:OG1	2.38	0.41
1:A:267:GLN:C	1:A:269:GLY:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:LEU:HD23	1:E:99:LEU:HD21	2.02	0.41
1:E:374:GLY:C	1:E:375:LYS:HD2	2.41	0.41
1:E:409:VAL:HG12	1:E:430:PRO:HA	2.02	0.41
1:F:294:ARG:O	1:F:298:GLN:HG3	2.21	0.41
1:G:6:TYR:CD2	1:G:73:ALA:HB2	2.56	0.41
1:J:213:LEU:O	1:J:217:ILE:HD12	2.20	0.41
1:A:8:PHE:CE2	1:A:163:MET:HG2	2.56	0.41
1:D:97:LYS:HE2	1:D:173:ARG:HH22	1.85	0.41
1:D:264:ALA:O	1:D:268:ASP:HB2	2.20	0.41
1:D:272:THR:O	1:D:315:ARG:HD3	2.21	0.41
1:E:64:LEU:HD23	1:E:64:LEU:HA	1.88	0.41
1:H:309:LYS:HD2	1:H:395:LEU:O	2.21	0.41
1:I:405:ILE:HA	1:I:473:VAL:HG13	2.02	0.41
1:L:189:VAL:HG11	1:L:447:ALA:HA	2.02	0.41
1:B:286:GLN:HG2	1:B:376:ASP:HB3	2.02	0.41
1:C:6:TYR:HB3	1:C:73:ALA:HB2	2.03	0.41
1:D:134:PHE:CB	1:F:189:VAL:HG22	2.51	0.41
1:E:331:MET:HG3	1:E:452:PHE:CB	2.51	0.41
1:F:302:PHE:CG	1:F:303:ALA:N	2.88	0.41
1:G:168:ALA:HB2	1:G:320:MET:HB3	2.02	0.41
1:H:294:ARG:O	1:H:298:GLN:HG3	2.19	0.41
1:I:366:ASP:O	1:I:379:ALA:HA	2.20	0.41
1:I:368:GLN:O	1:I:380:ARG:NH2	2.54	0.41
1:L:53:LEU:HD13	1:L:59:ILE:CD1	2.50	0.41
1:L:243:ARG:HG3	1:L:243:ARG:HH11	1.86	0.41
1:B:42:GLY:HA3	1:B:43:ASN:C	2.41	0.41
1:C:485:LYS:HG2	1:C:489:LYS:CE	2.49	0.41
1:D:38:GLN:OE1	1:D:47:LEU:N	2.31	0.41
1:E:332:GLU:HB2	1:E:349:HIS:HD2	1.86	0.41
1:F:331:MET:HB2	1:F:450:THR:O	2.21	0.41
1:J:392:ASN:HA	1:J:451:CYS:O	2.21	0.41
1:K:86:LYS:HA	1:K:89:ILE:HG13	2.02	0.41
1:K:365:LEU:HD13	1:K:366:ASP:N	2.36	0.41
1:B:7:GLU:HG2	1:B:46:VAL:HG23	2.02	0.41
1:B:402:PHE:CB	1:B:470:ILE:HD11	2.48	0.41
1:E:95:LEU:CD2	1:E:99:LEU:HD21	2.51	0.41
1:E:363:PRO:HB2	1:E:381:LEU:HD22	2.02	0.41
1:F:100:LEU:HD12	1:F:162:TRP:CG	2.56	0.41
1:I:81:THR:HG23	1:I:82:PHE:N	2.36	0.41
1:K:7:GLU:N	1:K:71:VAL:O	2.43	0.41
1:A:100:LEU:HD22	1:A:144:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:VAL:HA	1:C:78:TRP:O	2.20	0.41
1:C:115:ILE:HG22	1:C:119:PHE:CD2	2.55	0.41
1:D:236:TYR:CD2	1:D:381:LEU:HD21	2.55	0.41
1:I:333:ASP:OD1	1:I:333:ASP:N	2.53	0.41
1:J:453:SER:HB3	1:J:456:VAL:HG12	2.03	0.41
1:K:471:GLU:HB2	1:K:495:TRP:CD1	2.56	0.41
1:L:329:SER:OG	1:L:354:CYS:HB3	2.21	0.41
1:A:66:ALA:O	1:A:97:LYS:HD2	2.21	0.41
1:B:7:GLU:HG2	1:B:46:VAL:HG21	2.03	0.41
1:B:108:ARG:HE	1:B:108:ARG:HB2	1.46	0.41
1:C:1:MET:HB3	1:C:2:LYS:H	1.63	0.41
1:C:163:MET:O	1:C:167:VAL:HG23	2.20	0.41
1:C:292:VAL:O	1:C:296:MET:HG3	2.21	0.41
1:D:161:LYS:NZ	1:D:457:THR:HG21	2.36	0.41
1:D:272:THR:HB	1:D:315:ARG:HD3	2.03	0.41
1:E:407:ASN:HD21	1:E:437:SER:HB2	1.86	0.41
1:F:239:VAL:HG21	1:F:366:ASP:OD1	2.21	0.41
1:G:201:PHE:CE1	1:G:470:ILE:HD13	2.56	0.41
1:G:361:GLU:O	1:G:362:LYS:HD2	2.21	0.41
1:H:355:PRO:HA	1:H:383:PHE:CZ	2.56	0.41
1:I:178:ALA:HB2	1:I:271:PHE:CE1	2.56	0.41
1:I:320:MET:SD	1:I:460:GLN:HB3	2.61	0.41
1:I:332:GLU:OE1	1:I:449:HIS:NE2	2.54	0.41
1:I:413:LYS:HE3	1:I:413:LYS:HB2	1.80	0.41
1:J:102:LEU:HD22	1:J:104:THR:HB	2.02	0.41
1:J:102:LEU:CD2	1:J:104:THR:HB	2.50	0.41
1:J:303:ALA:HB3	1:J:307:ASP:O	2.21	0.41
1:K:135:ILE:HD12	1:K:135:ILE:HA	1.94	0.41
1:L:62:LEU:HA	1:L:62:LEU:HD12	1.77	0.41
1:L:287:LEU:HD12	1:L:288:PRO:HD2	2.03	0.41
1:A:345:VAL:O	1:A:427:LEU:HA	2.21	0.41
1:B:26:VAL:HG22	1:B:80:HIS:CD2	2.56	0.41
1:G:217:ILE:HD12	1:G:258:ILE:HA	2.01	0.41
1:B:30:ALA:O	1:B:34:VAL:HG23	2.22	0.40
1:B:113:ASP:HA	1:E:419:PRO:HD2	2.03	0.40
1:B:147:VAL:HG11	1:E:438:ALA:HB3	2.03	0.40
1:B:233:GLU:HG2	1:B:238:ILE:HD12	2.03	0.40
1:G:81:THR:HG22	1:G:122:LEU:O	2.21	0.40
1:G:325:GLN:O	1:G:325:GLN:HG2	2.22	0.40
1:I:149:HIS:ND1	1:I:151:GLU:HB2	2.37	0.40
1:I:248:VAL:HG22	1:I:367:VAL:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:303:ALA:HB3	1:L:307:ASP:O	2.21	0.40
1:C:372:ILE:HD11	1:E:18:TYR:HE1	1.85	0.40
1:D:152:ASP:O	1:D:155:VAL:HG22	2.22	0.40
1:F:286:GLN:HB3	1:F:378:PRO:HB3	2.03	0.40
1:I:213:LEU:HD11	1:I:262:LEU:HD23	2.03	0.40
1:A:336:TYR:HD1	1:A:345:VAL:HG22	1.87	0.40
1:A:355:PRO:HA	1:A:383:PHE:CZ	2.56	0.40
1:B:135:ILE:HG23	1:B:139:MET:HG3	2.04	0.40
1:C:349:HIS:O	1:C:423:VAL:HG11	2.21	0.40
1:D:336:TYR:CD1	1:D:345:VAL:HG12	2.56	0.40
1:E:362:LYS:HD2	1:E:362:LYS:H	1.85	0.40
1:F:254:GLU:OE1	1:F:257:ARG:NH1	2.55	0.40
1:G:90:ARG:HH12	1:I:173:ARG:HG3	1.86	0.40
1:I:314:LEU:HG	1:I:451:CYS:SG	2.61	0.40
1:I:344:LEU:HD11	1:I:427:LEU:HD22	2.03	0.40
1:J:61:ARG:NH1	1:J:64:LEU:HD23	2.36	0.40
1:J:289:GLY:O	1:J:293:GLN:HG2	2.21	0.40
1:K:34:VAL:CG1	1:K:35:PRO:HD3	2.52	0.40
1:L:100:LEU:HD12	1:L:162:TRP:CD2	2.56	0.40
1:D:372:ILE:N	1:D:372:ILE:HD12	2.37	0.40
1:E:320:MET:O	1:E:460:GLN:NE2	2.43	0.40
1:F:34:VAL:HB	1:F:35:PRO:HD3	2.03	0.40
1:F:139:MET:HE2	1:F:139:MET:HB3	1.95	0.40
1:F:337:HIS:HB3	1:F:344:LEU:HD12	2.04	0.40
1:K:290:LEU:CD1	1:K:365:LEU:HD21	2.51	0.40
1:B:84:PRO:O	1:B:87:MET:HE2	2.22	0.40
1:F:239:VAL:HG12	1:F:241:ALA:H	1.86	0.40
1:G:233:GLU:OE2	1:G:249:ARG:NH2	2.54	0.40
1:J:11:VAL:HG21	1:J:62:LEU:HD21	2.03	0.40
1:J:53:LEU:HB3	1:J:59:ILE:HG12	2.04	0.40
1:L:153:PRO:HA	1:L:156:ARG:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/498 (100%)	463 (93%)	24 (5%)	10 (2%)	7	30
1	B	495/498 (99%)	470 (95%)	22 (4%)	3 (1%)	25	57
1	C	496/498 (100%)	462 (93%)	24 (5%)	10 (2%)	7	30
1	D	496/498 (100%)	461 (93%)	29 (6%)	6 (1%)	13	41
1	E	495/498 (99%)	468 (94%)	23 (5%)	4 (1%)	19	51
1	F	494/498 (99%)	467 (94%)	23 (5%)	4 (1%)	19	51
1	G	496/498 (100%)	467 (94%)	24 (5%)	5 (1%)	15	46
1	H	495/498 (99%)	469 (95%)	20 (4%)	6 (1%)	13	41
1	I	496/498 (100%)	464 (94%)	22 (4%)	10 (2%)	7	30
1	J	496/498 (100%)	467 (94%)	23 (5%)	6 (1%)	13	41
1	K	496/498 (100%)	469 (95%)	23 (5%)	4 (1%)	19	51
1	L	494/498 (99%)	455 (92%)	25 (5%)	14 (3%)	5	24
All	All	5946/5976 (100%)	5582 (94%)	282 (5%)	82 (1%)	11	37

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	ALA
1	B	40	ALA
1	B	41	VAL
1	C	40	ALA
1	C	45	HIS
1	C	185	ARG
1	C	322	THR
1	D	41	VAL
1	E	40	ALA
1	E	324	LEU
1	E	325	GLN
1	F	51	GLY
1	G	40	ALA
1	H	42	GLY
1	H	322	THR
1	H	359	ALA
1	I	5	ALA
1	I	40	ALA
1	I	185	ARG

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Mol	Chain	Res	Type
1	I	340	LYS
1	I	359	ALA
1	J	41	VAL
1	K	40	ALA
1	L	5	ALA
1	L	41	VAL
1	L	43	ASN
1	L	326	GLY
1	L	359	ALA
1	A	19	GLY
1	A	340	LYS
1	C	5	ALA
1	C	359	ALA
1	D	324	LEU
1	G	19	GLY
1	H	40	ALA
1	I	41	VAL
1	J	51	GLY
1	L	51	GLY
1	L	241	ALA
1	L	324	LEU
1	L	340	LYS
1	A	20	ASP
1	A	269	GLY
1	B	44	ALA
1	C	43	ASN
1	C	340	LYS
1	D	51	GLY
1	D	340	LYS
1	F	45	HIS
1	F	325	GLN
1	F	340	LYS
1	G	20	ASP
1	J	40	ALA
1	L	40	ALA
1	L	240	PRO
1	L	362	LYS
1	A	268	ASP
1	G	44	ALA
1	H	39	ALA
1	I	341	GLY
1	J	126	ALA

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Mol	Chain	Res	Type
1	K	39	ALA
1	K	340	LYS
1	K	360	GLU
1	L	360	GLU
1	A	6	TYR
1	A	325	GLN
1	C	4	PRO
1	C	283	GLY
1	D	2	LYS
1	D	3	MET
1	E	326	GLY
1	H	299	GLY
1	I	17	LEU
1	I	219	ASP
1	A	5	ALA
1	A	4	PRO
1	J	42	GLY
1	L	341	GLY
1	G	51	GLY
1	I	4	PRO
1	J	323	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/405 (100%)	396 (98%)	10 (2%)	47	72
1	B	404/405 (100%)	395 (98%)	9 (2%)	52	75
1	C	405/405 (100%)	394 (97%)	11 (3%)	44	70
1	D	405/405 (100%)	393 (97%)	12 (3%)	41	68
1	E	404/405 (100%)	392 (97%)	12 (3%)	41	68
1	F	403/405 (100%)	396 (98%)	7 (2%)	60	80
1	G	405/405 (100%)	394 (97%)	11 (3%)	44	70
1	H	404/405 (100%)	395 (98%)	9 (2%)	52	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	405/405 (100%)	394 (97%)	11 (3%)	44	70
1	J	405/405 (100%)	398 (98%)	7 (2%)	60	80
1	K	405/405 (100%)	390 (96%)	15 (4%)	34	62
1	L	403/405 (100%)	395 (98%)	8 (2%)	55	77
All	All	4854/4860 (100%)	4732 (98%)	122 (2%)	47	72

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	70	ASP
1	A	79	MET
1	A	138	ARG
1	A	152	ASP
1	A	182	ASP
1	A	285	LYS
1	A	315	ARG
1	A	333	ASP
1	A	425	ARG
1	B	61	ARG
1	B	70	ASP
1	B	315	ARG
1	B	334	TYR
1	B	346	LEU
1	B	375	LYS
1	B	380	ARG
1	B	420	LYS
1	B	425	ARG
1	C	70	ASP
1	C	83	SER
1	C	138	ARG
1	C	224	LYS
1	C	362	LYS
1	C	366	ASP
1	C	368	GLN
1	C	380	ARG
1	C	394	SER
1	C	437	SER
1	C	451	CYS
1	D	55	ASP
1	D	61	ARG

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Mol	Chain	Res	Type
1	D	62	LEU
1	D	96	ARG
1	D	152	ASP
1	D	253	ARG
1	D	268	ASP
1	D	334	TYR
1	D	340	LYS
1	D	349	HIS
1	D	425	ARG
1	D	498	ARG
1	E	2	LYS
1	E	3	MET
1	E	20	ASP
1	E	120	MET
1	E	230	ASP
1	E	267	GLN
1	E	268	ASP
1	E	270	ASN
1	E	334	TYR
1	E	375	LYS
1	E	384	ASP
1	E	425	ARG
1	F	63	CYS
1	F	216	TYR
1	F	243	ARG
1	F	380	ARG
1	F	384	ASP
1	F	425	ARG
1	F	463	ASP
1	G	21	GLU
1	G	79	MET
1	G	138	ARG
1	G	215	GLN
1	G	249	ARG
1	G	263	LYS
1	G	268	ASP
1	G	315	ARG
1	G	333	ASP
1	G	384	ASP
1	G	425	ARG
1	H	54	LYS
1	H	61	ARG

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Mol	Chain	Res	Type
1	H	70	ASP
1	H	243	ARG
1	H	315	ARG
1	H	334	TYR
1	H	380	ARG
1	H	420	LYS
1	H	425	ARG
1	I	143	ARG
1	I	173	ARG
1	I	212	ASP
1	I	315	ARG
1	I	317	MET
1	I	333	ASP
1	I	334	TYR
1	I	366	ASP
1	I	394	SER
1	I	425	ARG
1	I	435	ARG
1	J	55	ASP
1	J	62	LEU
1	J	96	ARG
1	J	268	ASP
1	J	334	TYR
1	J	425	ARG
1	J	435	ARG
1	K	20	ASP
1	K	48	ARG
1	K	70	ASP
1	K	215	GLN
1	K	267	GLN
1	K	268	ASP
1	K	333	ASP
1	K	334	TYR
1	K	362	LYS
1	K	375	LYS
1	K	384	ASP
1	K	401	ARG
1	K	425	ARG
1	K	466	GLU
1	K	498	ARG
1	L	53	LEU
1	L	69	ASP

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Mol	Chain	Res	Type
1	L	138	ARG
1	L	182	ASP
1	L	216	TYR
1	L	333	ASP
1	L	380	ARG
1	L	425	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	B	124	GLN
1	C	101	HIS
1	D	45	HIS
1	E	124	GLN
1	E	255	GLN
1	E	286	GLN
1	E	449	HIS
1	F	286	GLN
1	J	16	HIS
1	K	491	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	498/498 (100%)	0.22	8 (1%) 72 70	25, 48, 76, 94	0
1	B	497/498 (99%)	0.16	7 (1%) 75 74	25, 48, 74, 95	0
1	C	498/498 (100%)	0.21	8 (1%) 72 70	25, 46, 75, 92	0
1	D	498/498 (100%)	0.33	11 (2%) 62 60	26, 49, 77, 95	0
1	E	497/498 (99%)	0.19	4 (0%) 86 85	26, 49, 77, 98	0
1	F	496/498 (99%)	0.23	5 (1%) 82 81	25, 51, 77, 103	0
1	G	498/498 (100%)	0.27	15 (3%) 50 49	26, 49, 81, 91	0
1	H	497/498 (99%)	0.28	8 (1%) 72 70	26, 50, 78, 96	0
1	I	498/498 (100%)	0.23	4 (0%) 86 85	24, 47, 77, 102	0
1	J	498/498 (100%)	0.23	6 (1%) 79 77	25, 48, 76, 91	0
1	K	498/498 (100%)	0.30	10 (2%) 65 64	26, 50, 80, 99	0
1	L	496/498 (99%)	0.29	13 (2%) 56 54	26, 50, 79, 105	0
All	All	5969/5976 (99%)	0.24	99 (1%) 70 68	24, 49, 78, 105	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	ASP	4.6
1	G	411	ALA	4.4
1	K	237	ASP	4.3
1	D	282	HIS	4.1
1	L	121	ASN	4.0
1	D	372	ILE	4.0
1	J	14	SER	3.6
1	L	221	SER	3.6
1	D	376	ASP	3.4
1	G	236	TYR	3.4
1	C	228	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	5	ALA	3.3
1	H	246	GLY	3.3
1	B	333	ASP	3.2
1	A	13	GLY	3.1
1	G	117	MET	3.1
1	H	232	TYR	3.0
1	L	219	ASP	3.0
1	G	219	ASP	2.9
1	K	329	SER	2.9
1	A	1	MET	2.9
1	G	116	ASP	2.9
1	L	280	ASP	2.9
1	A	218	ARG	2.9
1	I	498	ARG	2.9
1	K	497	GLY	2.9
1	G	209	GLY	2.8
1	J	428	TRP	2.8
1	A	124	GLN	2.8
1	D	4	PRO	2.8
1	F	4	PRO	2.8
1	C	152	ASP	2.8
1	I	221	SER	2.7
1	C	384	ASP	2.6
1	L	109	ASP	2.6
1	G	235	LEU	2.6
1	B	379	ALA	2.6
1	K	451	CYS	2.6
1	H	368	GLN	2.6
1	C	371	GLY	2.6
1	A	426	ILE	2.6
1	B	188	ALA	2.6
1	J	451	CYS	2.5
1	J	114	THR	2.5
1	G	223	GLN	2.5
1	E	62	LEU	2.5
1	A	159	LEU	2.4
1	H	333	ASP	2.4
1	D	109	ASP	2.4
1	F	20	ASP	2.4
1	G	451	CYS	2.4
1	I	451	CYS	2.3
1	D	247	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	371	GLY	2.3
1	G	352	GLU	2.3
1	L	223	GLN	2.3
1	D	339	GLU	2.3
1	D	361	GLU	2.3
1	G	4	PRO	2.3
1	E	280	ASP	2.3
1	K	14	SER	2.3
1	K	359	ALA	2.3
1	L	55	ASP	2.3
1	F	43	ASN	2.2
1	F	70	ASP	2.2
1	J	434	LEU	2.2
1	L	397	ASP	2.2
1	A	377	ASP	2.2
1	G	220	VAL	2.2
1	H	193	ASP	2.2
1	A	12	VAL	2.2
1	K	377	ASP	2.2
1	B	58	GLU	2.2
1	B	386	GLY	2.2
1	K	192	GLY	2.2
1	G	188	ALA	2.2
1	L	18	TYR	2.2
1	H	376	ASP	2.1
1	C	280	ASP	2.1
1	H	120	MET	2.1
1	K	367	VAL	2.1
1	C	109	ASP	2.1
1	C	366	ASP	2.1
1	J	221	SER	2.1
1	B	193	ASP	2.1
1	G	354	CYS	2.1
1	H	307	ASP	2.1
1	E	372	ILE	2.1
1	G	221	SER	2.1
1	F	424	ALA	2.0
1	D	17	LEU	2.0
1	L	343	ASP	2.0
1	L	450	THR	2.0
1	D	397	ASP	2.0
1	L	338	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	255	GLN	2.0
1	C	14	SER	2.0
1	D	110	ILE	2.0
1	K	253	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

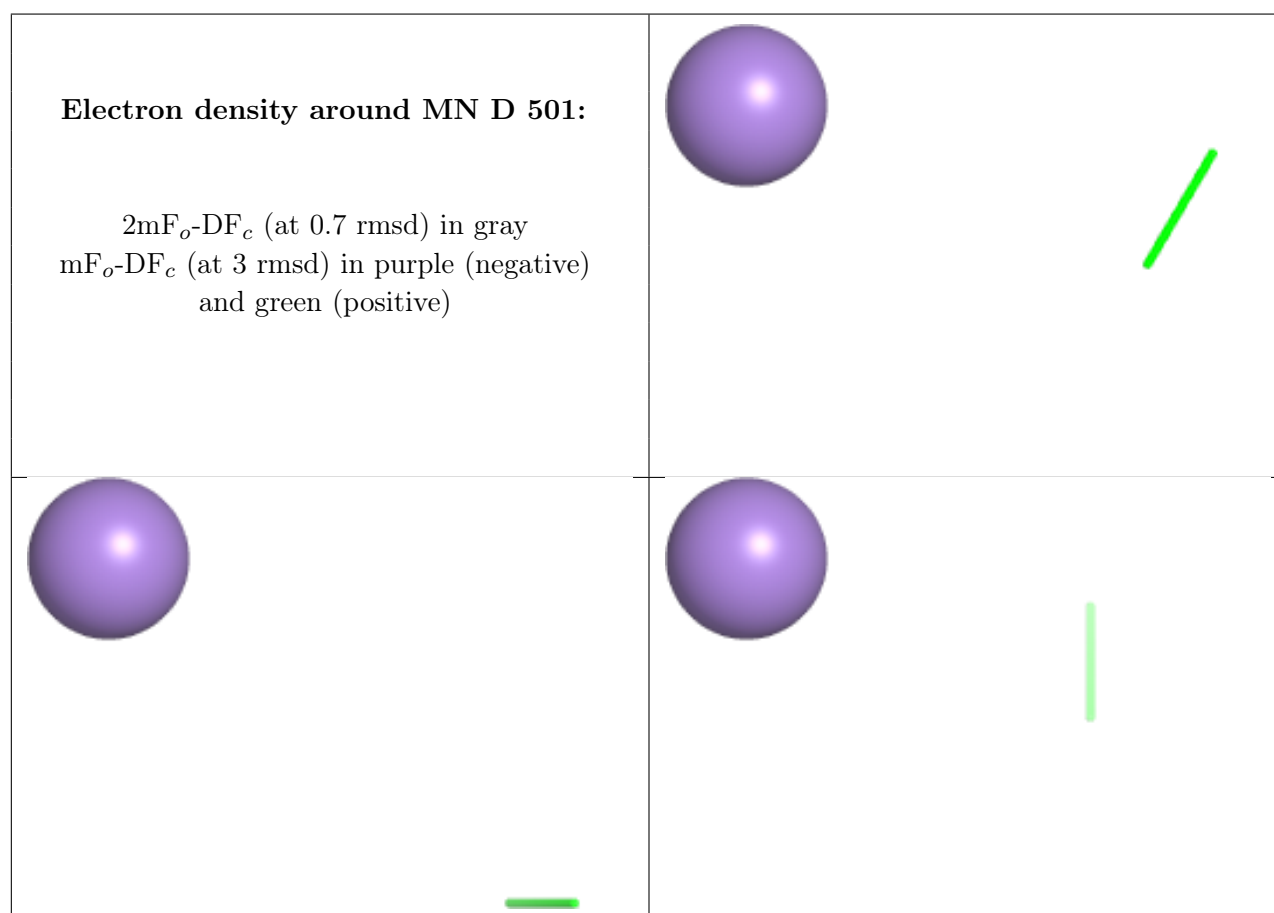
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	D	502	1/1	0.73	0.26	39,39,39,39	0
3	NA	F	502	1/1	0.83	0.28	39,39,39,39	0
3	NA	K	502	1/1	0.83	0.31	35,35,35,35	0
3	NA	I	502	1/1	0.84	0.17	29,29,29,29	0
3	NA	C	502	1/1	0.84	0.32	25,25,25,25	0
2	MN	D	501	1/1	0.90	0.10	48,48,48,48	0
3	NA	B	502	1/1	0.91	0.35	28,28,28,28	0
3	NA	G	502	1/1	0.91	0.32	31,31,31,31	0
3	NA	E	502	1/1	0.92	0.21	29,29,29,29	0
2	MN	A	501	1/1	0.93	0.09	54,54,54,54	0
2	MN	E	501	1/1	0.93	0.17	73,73,73,73	0
2	MN	J	501	1/1	0.93	0.10	50,50,50,50	0
3	NA	A	502	1/1	0.93	0.30	35,35,35,35	0
2	MN	L	501	1/1	0.94	0.07	54,54,54,54	0
3	NA	J	502	1/1	0.94	0.27	38,38,38,38	0
2	MN	H	501	1/1	0.94	0.04	44,44,44,44	0
3	NA	L	502	1/1	0.94	0.49	40,40,40,40	0
2	MN	K	501	1/1	0.95	0.08	61,61,61,61	0
2	MN	C	501	1/1	0.95	0.09	49,49,49,49	0

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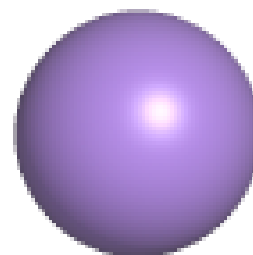
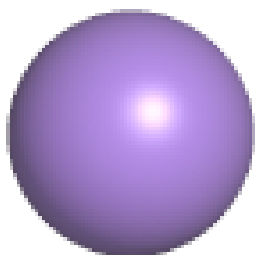
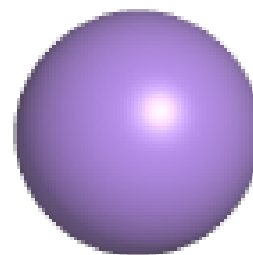
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	G	501	1/1	0.95	0.06	53,53,53,53	0
3	NA	H	502	1/1	0.95	0.36	26,26,26,26	0
2	MN	B	501	1/1	0.96	0.12	42,42,42,42	0
2	MN	I	501	1/1	0.97	0.04	45,45,45,45	0
2	MN	F	501	1/1	0.97	0.06	46,46,46,46	0

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.



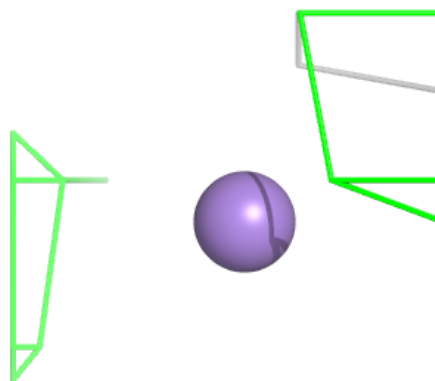
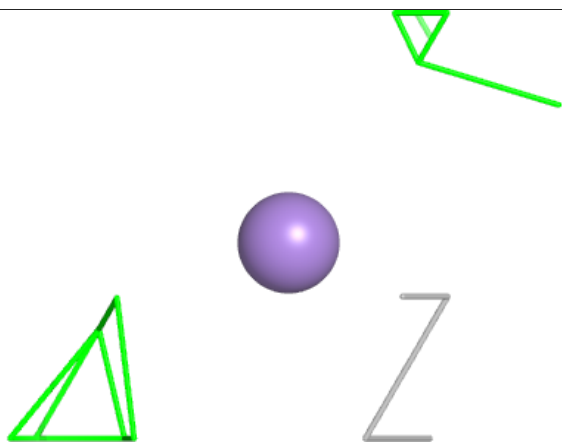
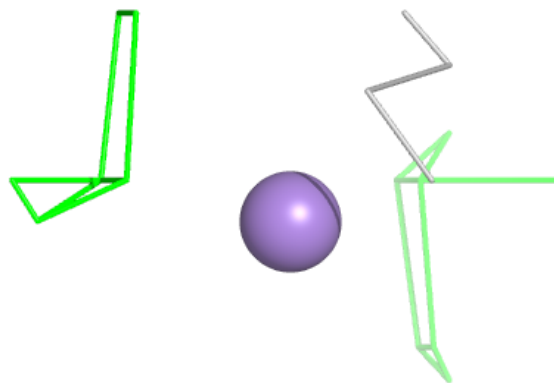
Electron density around MN A 501:

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

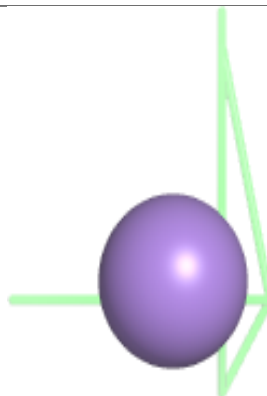


Electron density around MN E 501:

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

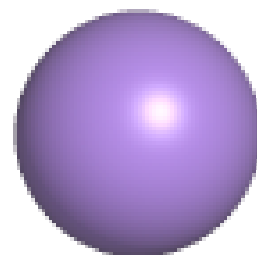
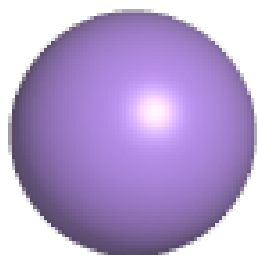
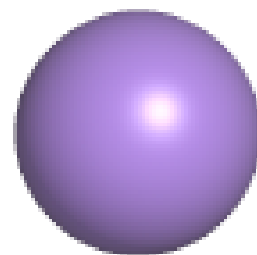
**Electron density around MN J 501:**

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



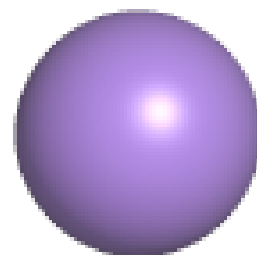
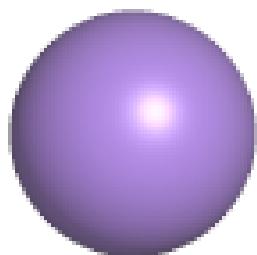
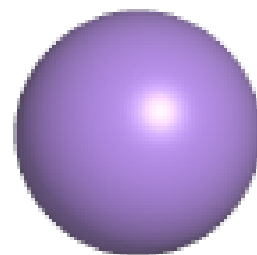
Electron density around MN L 501:

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



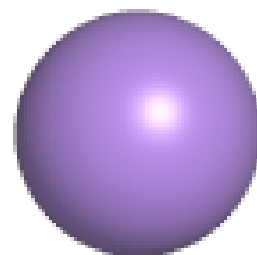
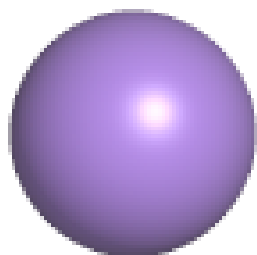
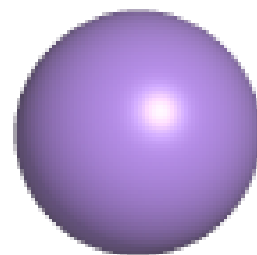
Electron density around MN H 501:

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



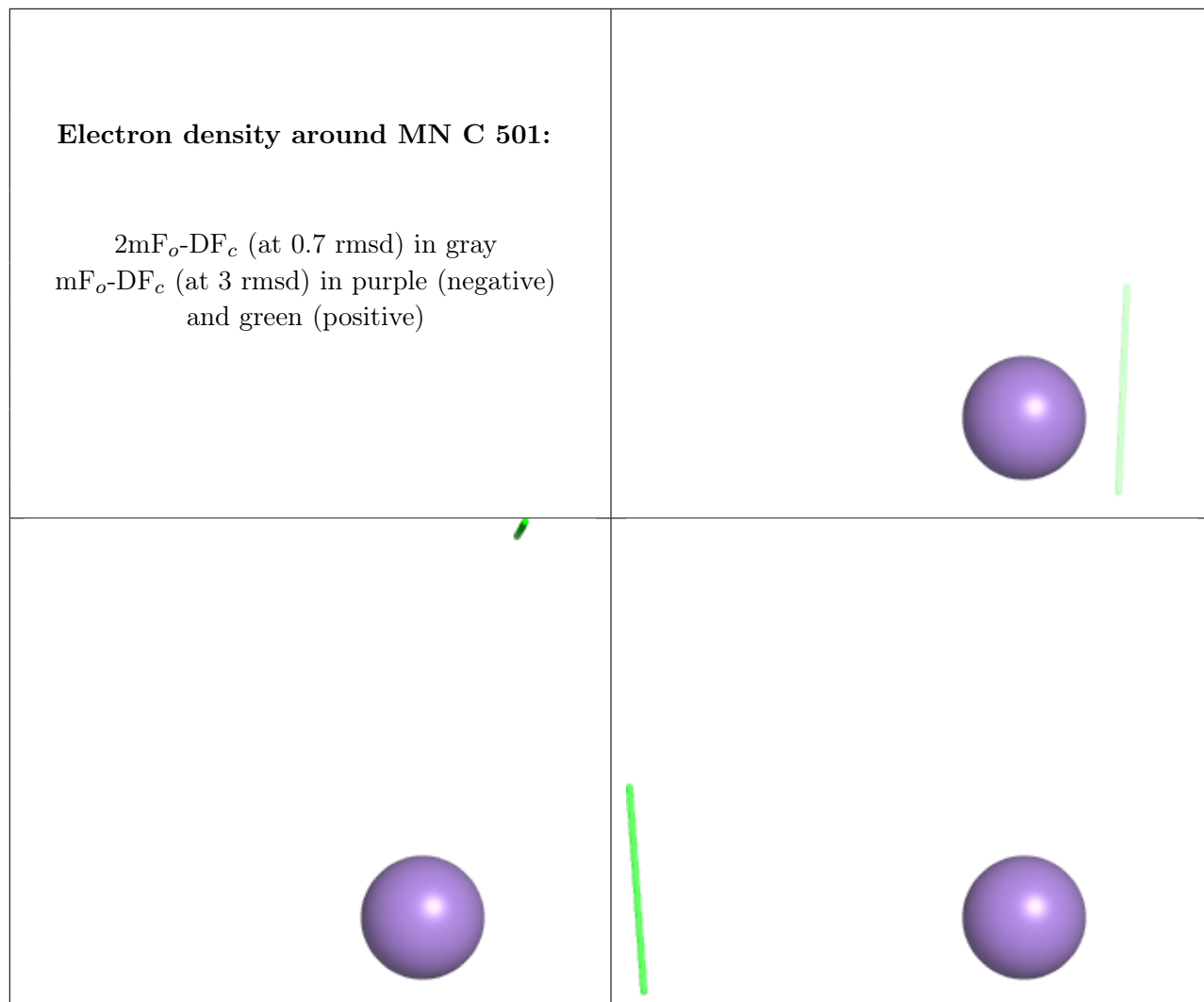
Electron density around MN K 501:

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



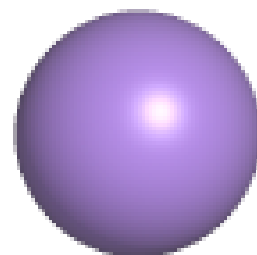
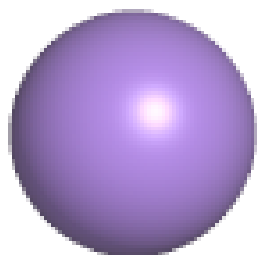
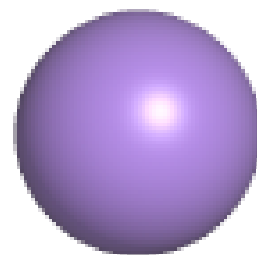
Electron density around MN C 501:

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



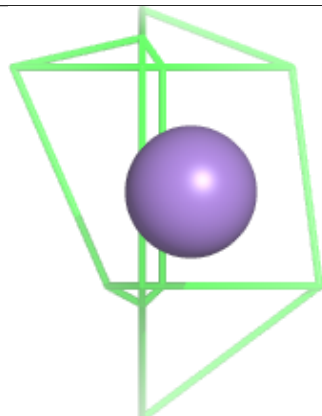
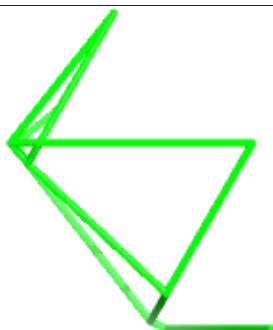
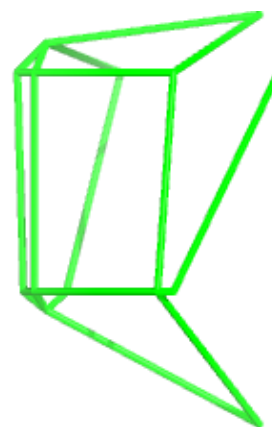
Electron density around MN G 501:

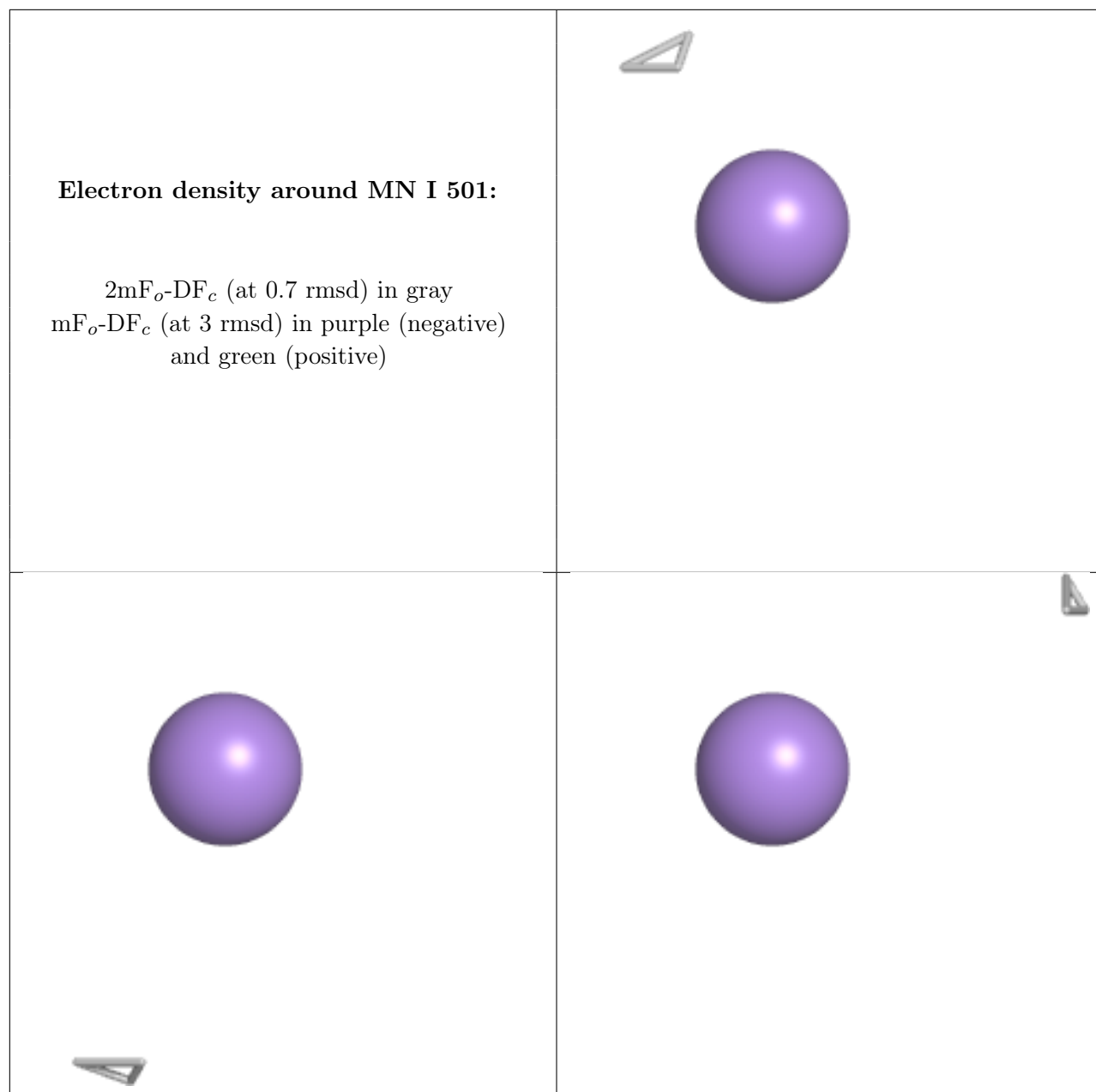
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

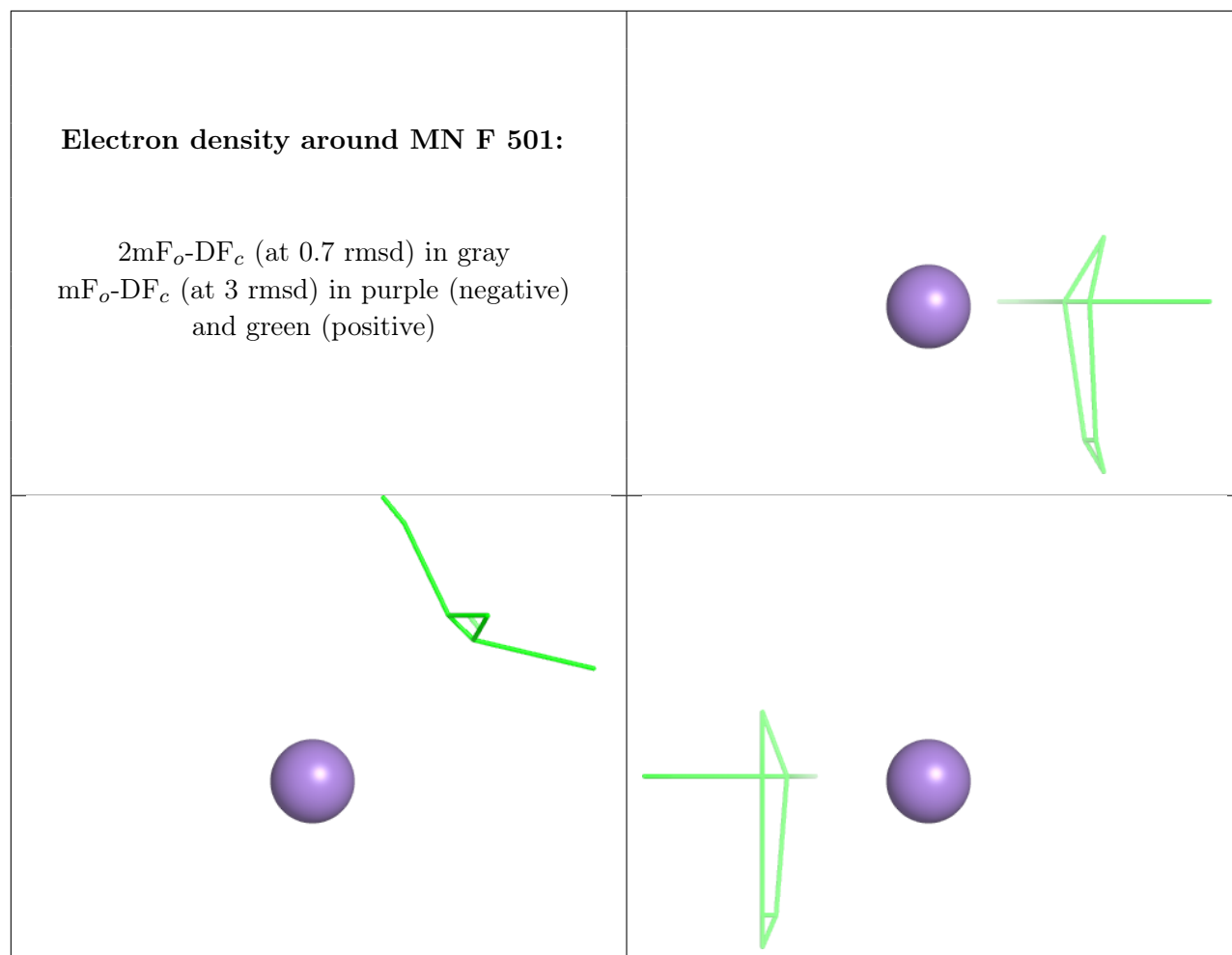


Electron density around MN B 501:

$2mF_o-DF_c$ (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.