



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 04:58 PM JST

PDB ID : 7CWV
Title : Crystal structure of Arabinose isomerase from hyper thermophilic bacterium *Thermotoga maritima* (TMAI) wt
Authors : Hoang, N.K.Q.; Dhanasingh, I.; Cao, T.P.; Sung, J.Y.; Shin, S.M.; Lee, D.W.; Lee, S.H.
Deposited on : 2020-08-31
Resolution : 3.53 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

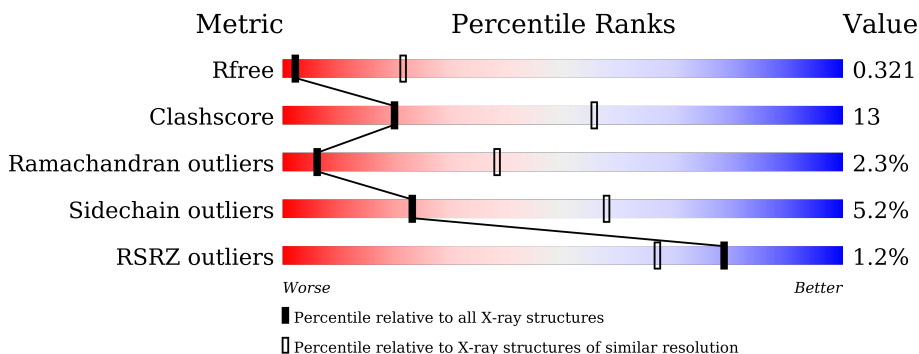
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 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	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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	496	 63% 33%
1	B	496	 70% 27%
1	C	496	 60% 37%
1	D	496	 67% 29%
1	E	496	 64% 33%

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Mol	Chain	Length	Quality of chain
1	F	496	 63% 34% .
1	G	496	 2% 68% 28% .
1	H	496	 % 68% 30% .
1	I	496	 2% 67% 31% .
1	J	496	 % 64% 33% .
1	K	496	 % 66% 31% .
1	L	496	 2% 72% 27% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 47714 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 L-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	491	Total 3943	C 2534	N 675	O 715	S 19	0	0	0
1	B	494	Total 3973	C 2552	N 678	O 725	S 18	0	0	0
1	C	487	Total 3930	C 2524	N 670	O 717	S 19	0	0	0
1	D	495	Total 3981	C 2557	N 679	O 726	S 19	0	0	0
1	E	495	Total 3981	C 2557	N 679	O 726	S 19	0	0	0
1	F	495	Total 3981	C 2557	N 679	O 726	S 19	0	0	0
1	G	495	Total 3981	C 2557	N 679	O 726	S 19	0	0	0
1	H	495	Total 3981	C 2557	N 679	O 726	S 19	0	0	0
1	I	495	Total 3981	C 2557	N 679	O 726	S 19	0	0	0
1	J	495	Total 3981	C 2557	N 679	O 726	S 19	0	0	0
1	K	495	Total 3981	C 2557	N 679	O 726	S 19	0	0	0
1	L	495	Total 3981	C 2557	N 679	O 726	S 19	0	0	0

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

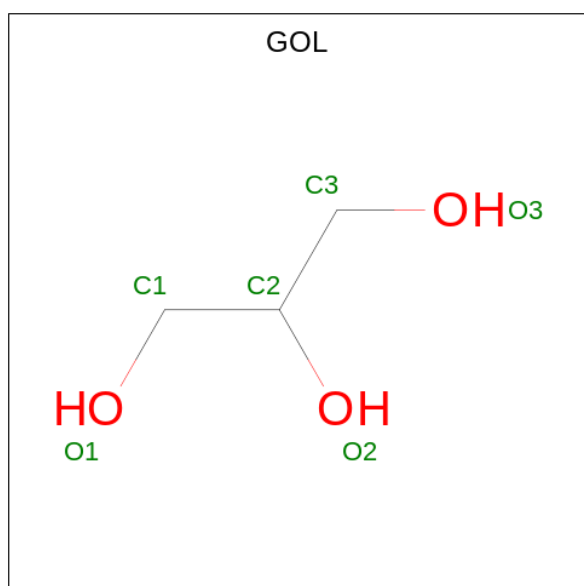
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		

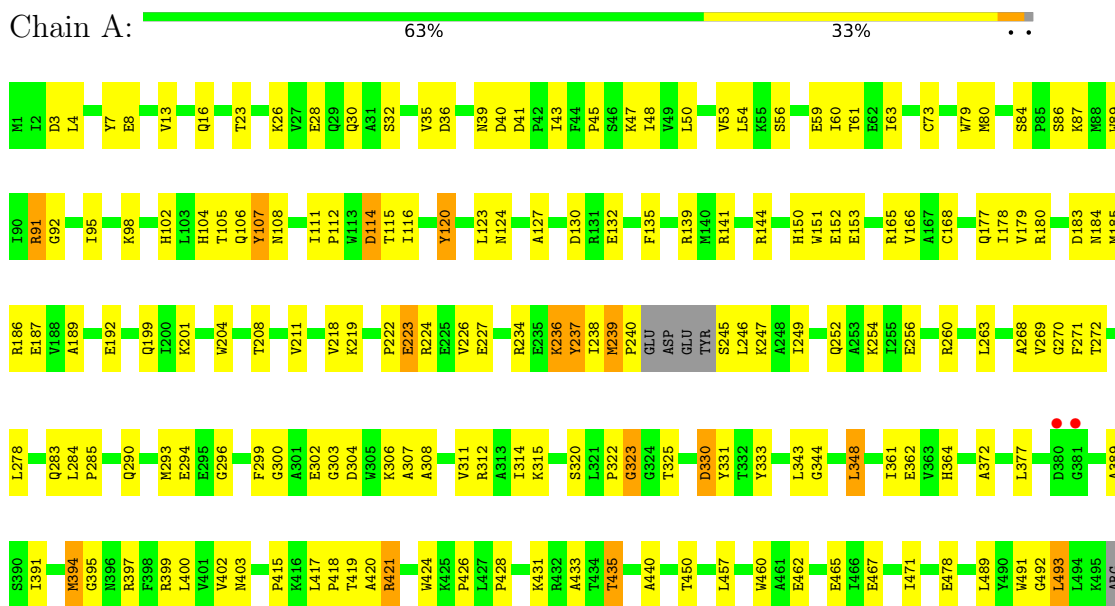
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0
4	F	2	Total O 2 2	0	0
4	G	4	Total O 4 4	0	0
4	H	1	Total O 1 1	0	0
4	I	1	Total O 1 1	0	0
4	J	2	Total O 2 2	0	0
4	K	2	Total O 2 2	0	0
4	L	1	Total O 1 1	0	0

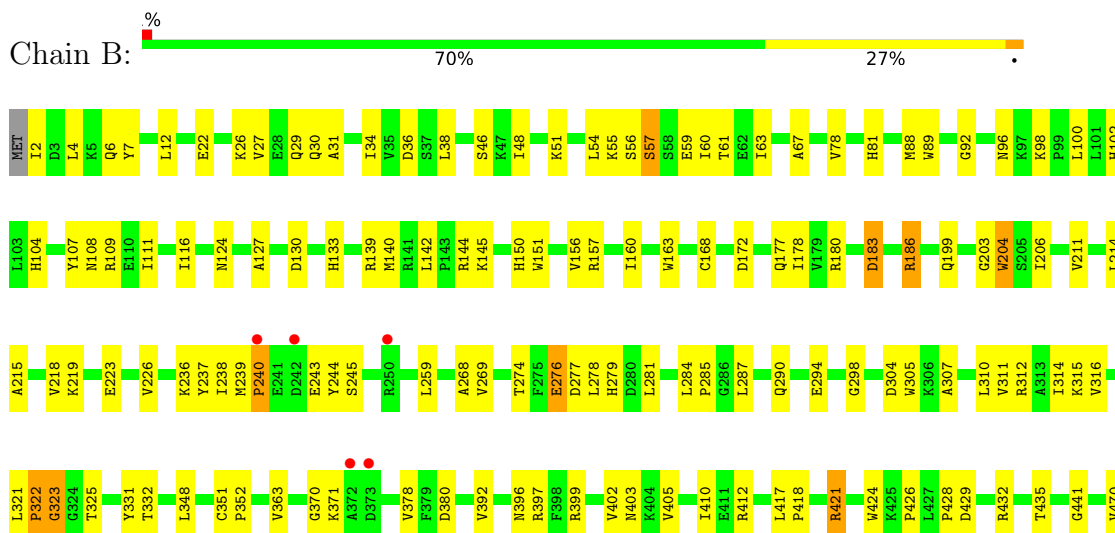
3 Residue-property plots

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

- Molecule 1: L-arabinose isomerase

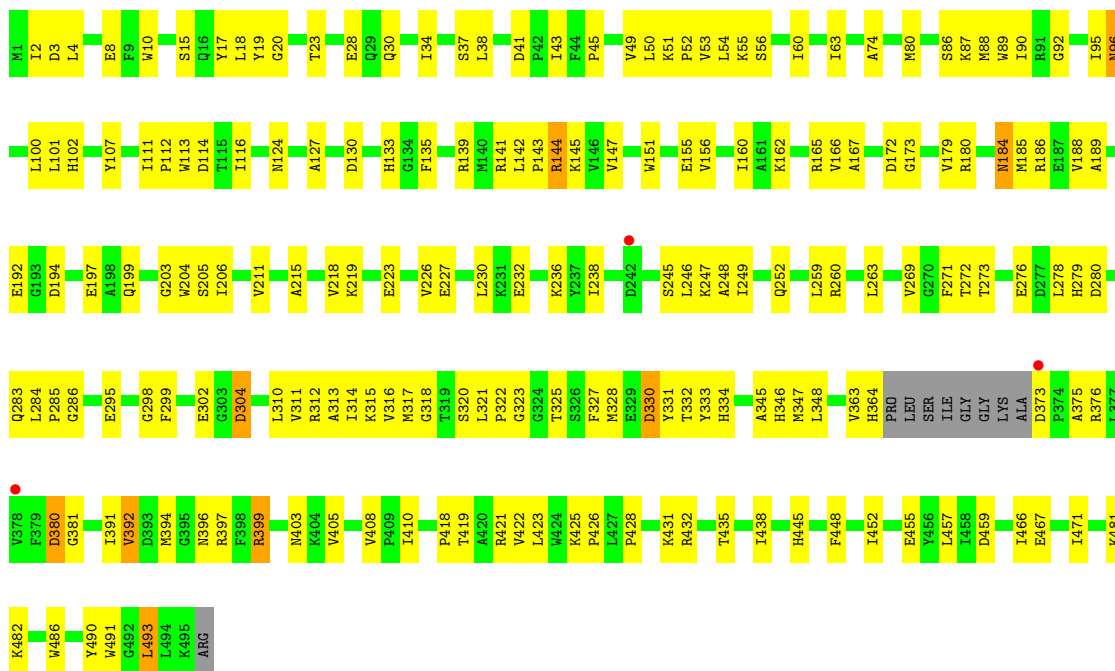


- Molecule 1: L-arabinose isomerase

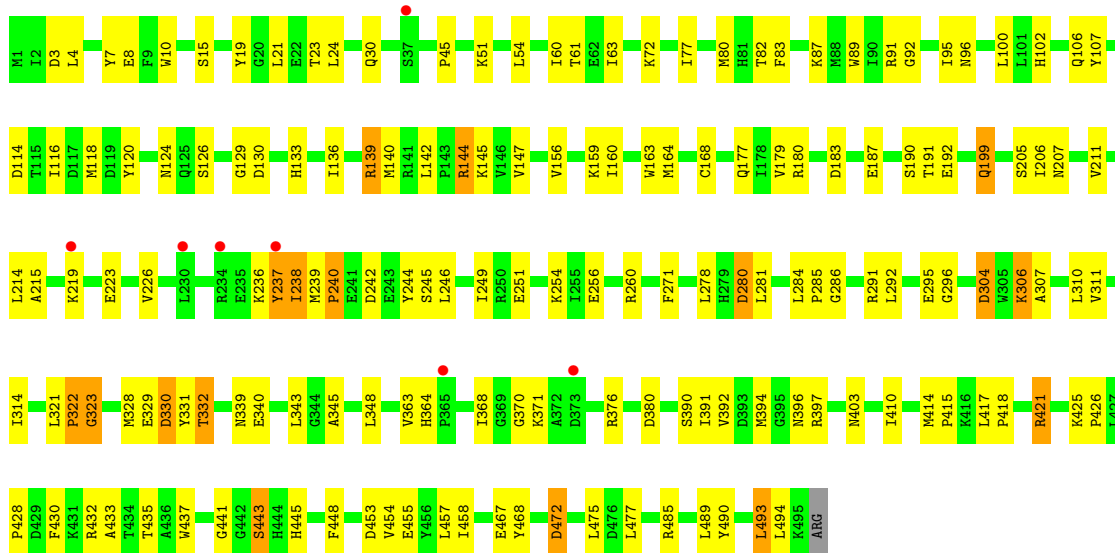




• Molecule 1: L-arabinose isomerase

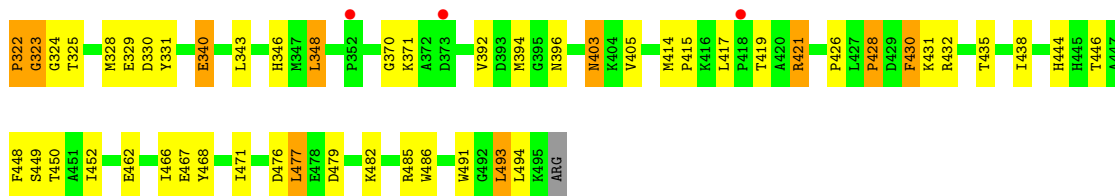


• Molecule 1: L-arabinose isomerase

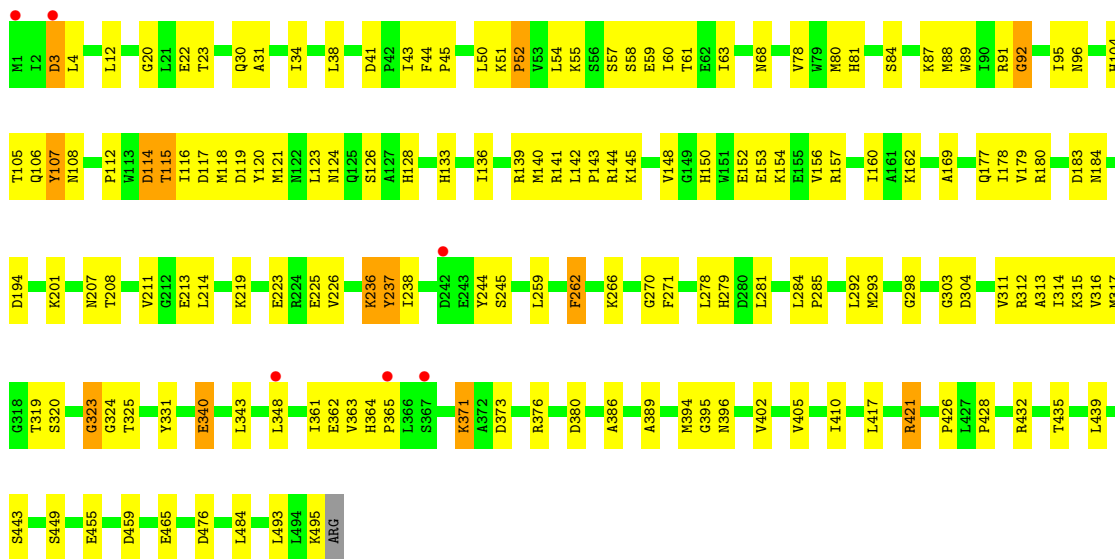


• Molecule 1: L-arabinose isomerase

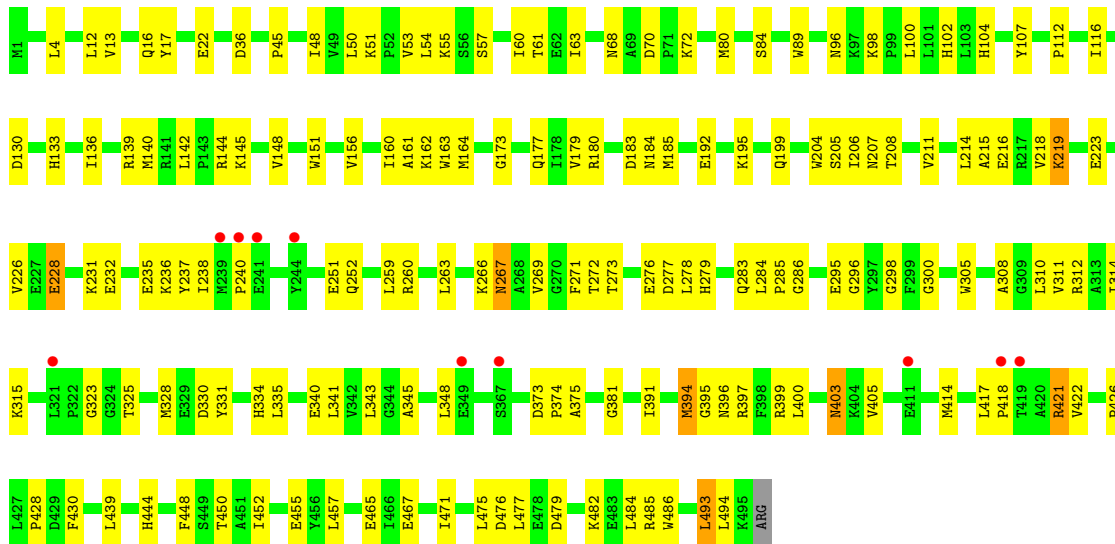




● Molecule 1: L-arabinose isomerase

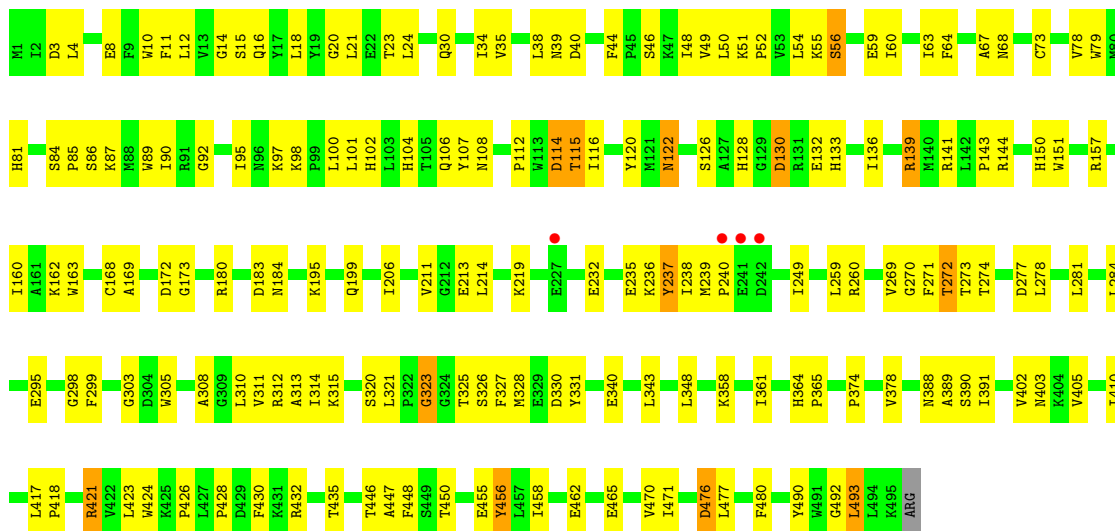


● Molecule 1: L-arabinose isomerase

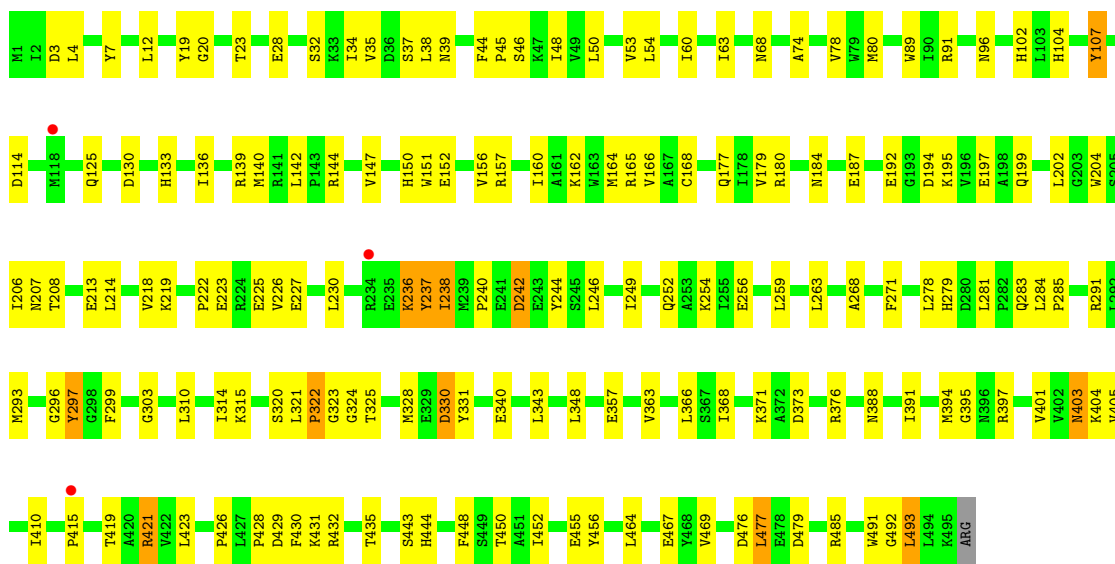


● Molecule 1: L-arabinose isomerase

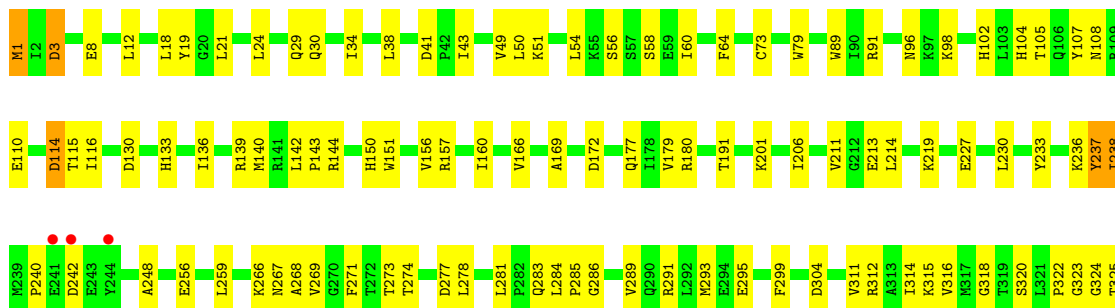


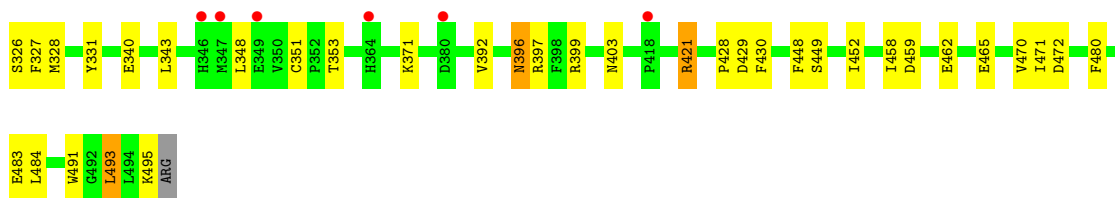


● Molecule 1: L-arabinose isomerase



● Molecule 1: L-arabinose isomerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	85.97Å 109.43Å 153.85Å 98.14° 98.18° 89.97°	Depositor
Resolution (Å)	49.74 – 3.53 49.70 – 3.53	Depositor EDS
% Data completeness (in resolution range)	91.6 (49.74-3.53) 91.6 (49.70-3.53)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.222 , 0.332 0.218 , 0.321	Depositor DCC
R_{free} test set	3146 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	88.6	Xtrriage
Anisotropy	0.064	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	47714	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, GOL

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	0.68	0/4036	0.82	0/5459
1	B	0.67	0/4068	0.79	0/5505
1	C	0.67	0/4023	0.81	0/5442
1	D	0.68	0/4076	0.81	0/5515
1	E	0.68	0/4076	0.80	0/5515
1	F	0.67	0/4076	0.81	0/5515
1	G	0.67	0/4076	0.82	0/5515
1	H	0.67	0/4076	0.80	0/5515
1	I	0.67	0/4076	0.80	0/5515
1	J	0.67	0/4076	0.79	0/5515
1	K	0.67	0/4076	0.79	0/5515
1	L	0.67	0/4076	0.79	0/5515
All	All	0.67	0/48811	0.80	0/66041

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3943	0	3971	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3973	0	3985	93	0
1	C	3930	0	3938	136	0
1	D	3981	0	3997	109	0
1	E	3981	0	3997	121	0
1	F	3981	0	3997	118	0
1	G	3981	0	3997	114	0
1	H	3981	0	3997	101	0
1	I	3981	0	3997	95	0
1	J	3981	0	3997	111	0
1	K	3981	0	3997	101	0
1	L	3981	0	3997	85	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	C	6	0	8	0	0
4	A	5	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	2	0	0	0	0
4	G	4	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	1	0	0	0	0
All	All	47714	0	47875	1201	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 13.

All (1201) 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:I:162:LYS:HD2	1:I:455:GLU:HG2	1.57	0.87
1:J:403:ASN:HD21	1:J:426:PRO:HB3	1.42	0.84
1:C:180:ARG:NH2	1:C:184:ASN:OD1	2.12	0.83
1:L:278:LEU:O	1:L:371:LYS:NZ	2.11	0.83
1:E:145:LYS:HD3	1:E:459:ASP:OD1	1.81	0.80
1:L:60:ILE:HG21	1:L:89:TRP:HA	1.64	0.78
1:B:322:PRO:O	1:B:323:GLY:O	2.00	0.78
1:K:252:GLN:NE2	1:K:283:GLN:OE1	2.17	0.78
1:F:444:HIS:HB2	1:G:128:HIS:HB2	1.67	0.77
1:D:177:GLN:OE1	1:D:207:ASN:ND2	2.18	0.76
1:I:251:GLU:OE1	1:I:283:GLN:HB3	1.87	0.75
1:A:239:MET:HB3	1:A:240:PRO:CD	2.16	0.74
1:H:12:LEU:HD11	1:H:63:ILE:HG21	1.70	0.73
1:B:403:ASN:HD21	1:B:426:PRO:HB3	1.53	0.73
1:H:194:ASP:OD2	1:J:139:ARG:NH1	2.20	0.73
1:A:239:MET:HB3	1:A:240:PRO:HD3	1.70	0.72
1:E:444:HIS:HB2	1:F:128:HIS:HB2	1.71	0.72
1:C:30:GLN:HG2	1:C:107:TYR:CD2	2.24	0.72
1:D:322:PRO:O	1:D:323:GLY:O	2.07	0.72
1:E:102:HIS:NE2	1:E:130:ASP:HB2	2.05	0.72
1:B:177:GLN:O	1:B:268:ALA:HA	1.89	0.71
1:L:211:VAL:HG11	1:L:278:LEU:HA	1.72	0.71
1:D:260:ARG:NH1	1:D:295:GLU:OE2	2.23	0.71
1:K:19:TYR:OH	1:K:125:GLN:OE1	2.06	0.70
1:B:278:LEU:O	1:B:371:LYS:NZ	2.25	0.70
1:E:39:ASN:HD21	1:E:48:ILE:HB	1.57	0.70
1:C:482:LYS:HB3	1:C:486:TRP:CH2	2.27	0.69
1:K:60:ILE:HG21	1:K:89:TRP:HA	1.75	0.69
1:I:199:GLN:HG2	1:I:204:TRP:O	1.93	0.69
1:A:290:GLN:NE2	1:A:348:LEU:O	2.26	0.69
1:C:107:TYR:HA	1:C:151:TRP:HE1	1.56	0.69
1:E:403:ASN:HA	1:E:471:ILE:HB	1.75	0.69
1:J:315:LYS:HD2	1:J:325:THR:HB	1.75	0.69
1:G:54:LEU:HD21	1:G:63:ILE:HG13	1.76	0.68
1:A:322:PRO:O	1:A:323:GLY:O	2.11	0.68
1:E:326:SER:OG	1:E:327:PHE:N	2.25	0.68
1:L:107:TYR:HA	1:L:151:TRP:HE1	1.58	0.68
1:B:60:ILE:HG21	1:B:89:TRP:HA	1.75	0.68
1:E:128:HIS:HB2	1:G:444:HIS:HB2	1.76	0.67
1:A:222:PRO:HG2	1:H:22:GLU:HG2	1.74	0.67
1:A:236:LYS:HB3	1:A:237:TYR:CD2	2.30	0.67
1:A:397:ARG:NH1	1:A:467:GLU:OE1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:ILE:HG21	1:F:89:TRP:HA	1.74	0.67
1:E:107:TYR:HA	1:E:151:TRP:HE1	1.59	0.67
1:A:60:ILE:HG21	1:A:89:TRP:HA	1.76	0.67
1:A:311:VAL:O	1:A:315:LYS:HB2	1.94	0.67
1:E:145:LYS:HE2	1:E:163:TRP:HB2	1.77	0.67
1:F:478:GLU:OE2	1:F:482:LYS:HE3	1.95	0.66
1:A:95:ILE:HD11	1:G:68:ASN:HB3	1.77	0.66
1:I:311:VAL:O	1:I:315:LYS:HB2	1.95	0.66
1:A:87:LYS:O	1:G:199:GLN:NE2	2.28	0.66
1:G:104:HIS:ND1	1:G:130:ASP:OD1	2.28	0.66
1:I:211:VAL:HG11	1:I:278:LEU:HA	1.78	0.66
1:K:199:GLN:HG2	1:K:204:TRP:O	1.96	0.66
1:L:133:HIS:O	1:L:136:ILE:HG22	1.96	0.66
1:A:218:VAL:HG23	1:A:254:LYS:HG2	1.78	0.66
1:E:269:VAL:HB	1:E:312:ARG:HG2	1.78	0.66
1:G:340:GLU:OE1	1:G:431:LYS:NZ	2.29	0.65
1:D:364:HIS:O	1:D:376:ARG:NH2	2.29	0.65
1:F:403:ASN:HA	1:F:471:ILE:HB	1.78	0.65
1:J:340:GLU:HG3	1:J:430:PHE:HB3	1.78	0.65
1:H:179:VAL:O	1:H:271:PHE:HA	1.96	0.65
1:J:85:PRO:HB3	1:K:187:GLU:O	1.96	0.65
1:E:60:ILE:HG21	1:E:89:TRP:HA	1.77	0.65
1:H:51:LYS:O	1:H:52:PRO:O	2.13	0.65
1:C:194:ASP:OD1	1:E:139:ARG:NH1	2.30	0.65
1:C:315:LYS:O	1:C:318:GLY:O	2.14	0.65
1:E:435:THR:HG23	1:E:477:LEU:HD21	1.79	0.65
1:A:236:LYS:HB3	1:A:237:TYR:CE2	2.32	0.65
1:H:211:VAL:HG11	1:H:278:LEU:HA	1.78	0.65
1:A:153:GLU:OE2	1:C:431:LYS:NZ	2.30	0.64
1:J:139:ARG:HH11	1:K:395:GLY:HA2	1.61	0.64
1:K:150:HIS:CE1	1:K:152:GLU:HG3	2.33	0.64
1:E:490:TYR:CE2	1:G:485:ARG:HD2	2.32	0.64
1:L:114:ASP:N	1:L:114:ASP:OD1	2.31	0.64
1:L:293:MET:O	1:L:315:LYS:NZ	2.30	0.64
1:G:60:ILE:HG21	1:G:89:TRP:HA	1.79	0.64
1:D:426:PRO:HG2	1:D:430:PHE:HD1	1.63	0.64
1:H:133:HIS:O	1:H:136:ILE:HG22	1.99	0.63
1:C:8:GLU:OE1	1:C:49:VAL:HG21	1.99	0.63
1:C:145:LYS:NZ	1:C:459:ASP:OD2	2.27	0.63
1:F:343:LEU:HD11	1:F:421:ARG:HB2	1.80	0.63
1:G:107:TYR:O	1:G:150:HIS:NE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:4:LEU:HD11	1:K:45:PRO:HB2	1.79	0.63
1:G:180:ARG:NH2	1:G:184:ASN:OD1	2.32	0.63
1:J:298:GLY:HA2	1:J:311:VAL:HG12	1.81	0.63
1:C:55:LYS:O	1:C:88:MET:SD	2.57	0.63
1:F:156:VAL:O	1:F:160:ILE:HG22	1.99	0.63
1:H:128:HIS:HB2	1:I:444:HIS:HB2	1.80	0.63
1:L:271:PHE:O	1:L:299:PHE:HA	2.00	0.62
1:I:183:ASP:OD1	1:I:184:ASN:ND2	2.32	0.62
1:H:259:LEU:HB3	1:H:292:LEU:HD21	1.81	0.62
1:L:104:HIS:ND1	1:L:130:ASP:OD2	2.32	0.62
1:B:214:LEU:HD11	1:B:259:LEU:HD22	1.81	0.62
1:C:206:ILE:O	1:E:87:LYS:NZ	2.24	0.62
1:B:211:VAL:HG11	1:B:278:LEU:HA	1.82	0.61
1:D:417:LEU:HD23	1:D:421:ARG:HE	1.65	0.61
1:B:104:HIS:CE1	1:B:130:ASP:OD1	2.53	0.61
1:C:245:SER:HA	1:C:363:VAL:HG21	1.82	0.61
1:F:4:LEU:HD11	1:F:45:PRO:HB2	1.82	0.61
1:G:405:VAL:HG12	1:G:426:PRO:HA	1.82	0.61
1:D:310:LEU:HD22	1:D:391:ILE:HG13	1.81	0.61
1:I:60:ILE:HG21	1:I:89:TRP:HA	1.83	0.61
1:K:147:VAL:HG12	1:K:156:VAL:HG23	1.83	0.61
1:L:311:VAL:HG21	1:L:327:PHE:HB2	1.83	0.61
1:I:403:ASN:HA	1:I:471:ILE:HB	1.82	0.61
1:A:293:MET:O	1:A:294:GLU:C	2.39	0.61
1:C:199:GLN:HG2	1:C:204:TRP:O	2.01	0.61
1:B:26:LYS:NZ	1:F:115:THR:OG1	2.34	0.61
1:F:184:ASN:HA	1:F:303:GLY:HA3	1.83	0.61
1:H:394:MET:O	1:H:396:ASN:OD1	2.19	0.61
1:H:417:LEU:HD23	1:H:421:ARG:HE	1.65	0.61
1:I:12:LEU:HD11	1:I:63:ILE:HG21	1.83	0.61
1:J:114:ASP:HA	1:K:415:PRO:HD2	1.83	0.61
1:K:102:HIS:NE2	1:K:130:ASP:HB2	2.15	0.61
1:L:150:HIS:O	1:L:156:VAL:HG11	2.01	0.60
1:L:227:GLU:HA	1:L:230:LEU:HB2	1.83	0.60
1:D:80:MET:CG	1:D:130:ASP:HB3	2.32	0.60
1:J:60:ILE:HG21	1:J:89:TRP:HA	1.84	0.60
1:J:403:ASN:HA	1:J:471:ILE:HB	1.83	0.60
1:E:476:ASP:HB3	1:E:479:ASP:HB2	1.83	0.60
1:J:184:ASN:HA	1:J:303:GLY:HA3	1.83	0.60
1:E:116:ILE:HD12	1:E:116:ILE:O	2.01	0.60
1:J:260:ARG:NH1	1:J:295:GLU:OE1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ILE:HG21	1:C:89:TRP:HA	1.84	0.60
1:I:68:ASN:OD1	1:I:96:ASN:HA	2.02	0.60
1:F:30:GLN:HG2	1:F:107:TYR:CD2	2.37	0.60
1:J:211:VAL:HG11	1:J:278:LEU:HA	1.84	0.60
1:L:311:VAL:O	1:L:315:LYS:HB2	2.01	0.60
1:C:102:HIS:NE2	1:C:130:ASP:HB2	2.17	0.59
1:L:64:PHE:HD1	1:L:96:ASN:HD22	1.50	0.59
1:L:266:LYS:O	1:L:268:ALA:N	2.35	0.59
1:D:54:LEU:HD21	1:D:63:ILE:HG13	1.85	0.59
1:H:405:VAL:HG12	1:H:426:PRO:HA	1.85	0.59
1:L:79:TRP:NE1	1:L:105:THR:O	2.35	0.59
1:H:114:ASP:OD1	1:H:114:ASP:N	2.35	0.59
1:I:185:MET:HG3	1:I:276:GLU:OE1	2.02	0.59
1:G:112:PRO:O	1:G:116:ILE:HG13	2.02	0.59
1:I:400:LEU:HD21	1:I:457:LEU:HD22	1.84	0.59
1:L:179:VAL:O	1:L:271:PHE:HA	2.03	0.59
1:I:343:LEU:HD11	1:I:421:ARG:HB2	1.84	0.59
1:K:54:LEU:HD13	1:K:60:ILE:HA	1.84	0.59
1:B:396:ASN:HB3	1:L:396:ASN:HB3	1.85	0.59
1:D:147:VAL:HG12	1:D:156:VAL:HG23	1.85	0.59
1:F:417:LEU:HB2	1:G:116:ILE:HD13	1.84	0.59
1:G:322:PRO:O	1:G:323:GLY:O	2.20	0.59
1:D:130:ASP:HA	1:D:133:HIS:HB3	1.85	0.58
1:E:141:ARG:HH22	1:G:394:MET:HB3	1.68	0.58
1:E:214:LEU:HD23	1:E:281:LEU:HD11	1.84	0.58
1:L:108:ASN:ND2	1:L:110:GLU:O	2.34	0.58
1:D:417:LEU:HD12	1:D:418:PRO:HD2	1.84	0.58
1:H:365:PRO:HA	1:H:373:ASP:HB3	1.83	0.58
1:G:3:ASP:OD1	1:G:4:LEU:N	2.36	0.58
1:G:476:ASP:HB3	1:G:479:ASP:HB2	1.86	0.58
1:J:410:ILE:HG13	1:J:423:LEU:HD12	1.86	0.58
1:B:107:TYR:HA	1:B:151:TRP:HE1	1.69	0.58
1:D:251:GLU:HA	1:D:254:LYS:HE3	1.85	0.58
1:I:283:GLN:NE2	1:I:374:PRO:HA	2.18	0.58
1:I:314:ILE:HD11	1:I:452:ILE:HD11	1.86	0.58
1:B:54:LEU:HD21	1:B:63:ILE:HG13	1.85	0.58
1:F:55:LYS:O	1:F:88:MET:SD	2.61	0.58
1:F:179:VAL:O	1:F:271:PHE:HA	2.04	0.58
1:F:340:GLU:HG3	1:F:430:PHE:HB3	1.84	0.58
1:K:12:LEU:HD11	1:K:63:ILE:HG21	1.85	0.58
1:L:397:ARG:HD2	1:L:491:TRP:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:ALA:O	1:F:218:VAL:HG22	2.03	0.58
1:K:78:VAL:HG11	1:K:133:HIS:CE1	2.39	0.58
1:L:21:LEU:HD12	1:L:24:LEU:HD12	1.86	0.58
1:A:201:LYS:HE3	1:A:465:GLU:O	2.04	0.57
1:G:178:ILE:HA	1:G:270:GLY:O	2.04	0.57
1:K:284:LEU:HD12	1:K:285:PRO:HD2	1.86	0.57
1:E:485:ARG:HB2	1:F:490:TYR:CG	2.39	0.57
1:K:68:ASN:HD21	1:K:96:ASN:HA	1.69	0.57
1:A:4:LEU:HD11	1:A:45:PRO:HB2	1.85	0.57
1:A:35:VAL:O	1:A:39:ASN:ND2	2.37	0.57
1:D:102:HIS:NE2	1:D:130:ASP:HB2	2.19	0.57
1:C:260:ARG:NH1	1:C:295:GLU:OE1	2.37	0.57
1:K:476:ASP:O	1:K:479:ASP:N	2.38	0.57
1:D:223:GLU:O	1:D:226:VAL:HG22	2.04	0.57
1:D:328:MET:HB2	1:D:448:PHE:HB2	1.86	0.57
1:F:133:HIS:O	1:F:136:ILE:HG22	2.04	0.57
1:C:165:ARG:HD3	1:C:317:MET:O	2.04	0.57
1:C:199:GLN:O	1:C:203:GLY:HA2	2.05	0.57
1:G:166:VAL:HG22	1:G:317:MET:SD	2.45	0.57
1:H:213:GLU:OE2	1:K:279:HIS:NE2	2.38	0.57
1:E:2:ILE:HD12	1:E:312:ARG:HH22	1.69	0.57
1:C:30:GLN:OE1	1:C:107:TYR:HB2	2.04	0.57
1:H:51:LYS:O	1:H:52:PRO:C	2.41	0.57
1:H:57:SER:O	1:H:61:THR:HG23	2.04	0.57
1:H:87:LYS:O	1:J:199:GLN:NE2	2.38	0.57
1:A:23:THR:OG1	1:A:123:LEU:HD12	2.05	0.57
1:D:60:ILE:HG21	1:D:89:TRP:HA	1.87	0.57
1:A:92:GLY:O	1:A:95:ILE:HG22	2.05	0.56
1:B:432:ARG:O	1:B:435:THR:HG22	2.04	0.56
1:D:340:GLU:HG3	1:D:430:PHE:HB3	1.86	0.56
1:G:320:SER:O	1:G:323:GLY:N	2.36	0.56
1:J:458:ILE:O	1:J:462:GLU:HB2	2.05	0.56
1:A:418:PRO:HG3	1:D:118:MET:HG2	1.86	0.56
1:D:179:VAL:O	1:D:271:PHE:HA	2.04	0.56
1:E:402:VAL:HG13	1:E:470:VAL:HA	1.87	0.56
1:H:116:ILE:HD11	1:I:414:MET:HG2	1.88	0.56
1:H:214:LEU:HD23	1:H:281:LEU:HD11	1.86	0.56
1:I:310:LEU:HD22	1:I:391:ILE:HG13	1.88	0.56
1:G:278:LEU:O	1:G:371:LYS:NZ	2.39	0.56
1:J:20:GLY:O	1:J:23:THR:HG22	2.05	0.56
1:A:184:ASN:HA	1:A:303:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:GLU:HB3	1:A:364:HIS:NE2	2.21	0.56
1:D:211:VAL:HG11	1:D:278:LEU:HA	1.88	0.56
1:F:427:LEU:O	1:F:433:ALA:HB2	2.06	0.56
1:K:278:LEU:O	1:K:281:LEU:HB2	2.06	0.56
1:C:74:ALA:O	1:C:167:ALA:HB1	2.06	0.56
1:G:3:ASP:OD1	1:G:3:ASP:C	2.44	0.56
1:H:92:GLY:O	1:H:95:ILE:HG22	2.06	0.56
1:B:104:HIS:ND1	1:B:130:ASP:OD1	2.39	0.56
1:B:27:VAL:HG13	1:B:81:HIS:CG	2.41	0.55
1:A:314:ILE:HG23	1:A:325:THR:HG21	1.87	0.55
1:C:223:GLU:O	1:C:226:VAL:HG22	2.06	0.55
1:B:180:ARG:HD2	1:B:206:ILE:HD11	1.86	0.55
1:G:201:LYS:HE2	1:G:466:ILE:HG22	1.89	0.55
1:J:328:MET:HB2	1:J:448:PHE:HB2	1.88	0.55
1:L:286:GLY:O	1:L:289:VAL:N	2.35	0.55
1:E:162:LYS:HD2	1:E:455:GLU:HG2	1.88	0.55
1:G:102:HIS:NE2	1:G:130:ASP:HB2	2.21	0.55
1:G:60:ILE:HG22	1:G:92:GLY:HA3	1.88	0.55
1:B:172:ASP:OD2	1:B:312:ARG:NE	2.36	0.55
1:E:438:ILE:HG23	1:F:134:GLY:HA3	1.89	0.55
1:F:414:MET:HB3	1:G:116:ILE:HD11	1.87	0.55
1:K:263:LEU:HD21	1:K:271:PHE:HB3	1.88	0.55
1:B:27:VAL:HG13	1:B:81:HIS:CD2	2.41	0.55
1:C:396:ASN:HB3	1:G:396:ASN:HB3	1.89	0.55
1:E:211:VAL:HG11	1:E:278:LEU:HA	1.87	0.55
1:F:321:LEU:C	1:F:323:GLY:H	2.09	0.55
1:G:324:GLY:O	1:G:450:THR:N	2.37	0.55
1:I:493:LEU:HG	1:I:494:LEU:H	1.71	0.55
1:L:30:GLN:HG2	1:L:107:TYR:CD2	2.41	0.55
1:C:310:LEU:HD22	1:C:391:ILE:HG13	1.89	0.55
1:C:405:VAL:HG12	1:C:426:PRO:HA	1.88	0.55
1:G:184:ASN:ND2	1:G:192:GLU:HG2	2.20	0.55
1:J:78:VAL:HG11	1:J:133:HIS:NE2	2.22	0.55
1:K:493:LEU:H	1:K:493:LEU:HD23	1.70	0.55
1:I:199:GLN:NE2	1:I:205:SER:HA	2.21	0.55
1:I:399:ARG:NE	1:I:467:GLU:OE1	2.40	0.55
1:E:284:LEU:HD12	1:E:285:PRO:HD2	1.89	0.54
1:I:260:ARG:NH1	1:I:295:GLU:OE2	2.40	0.54
1:G:165:ARG:HD3	1:G:317:MET:O	2.08	0.54
1:H:162:LYS:HD2	1:H:455:GLU:HG2	1.88	0.54
1:K:28:GLU:HG2	1:K:53:VAL:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:177:GLN:O	1:K:268:ALA:HA	2.07	0.54
1:E:102:HIS:HB3	1:E:146:VAL:HG22	1.88	0.54
1:H:278:LEU:O	1:H:371:LYS:NZ	2.32	0.54
1:I:130:ASP:HA	1:I:133:HIS:HB3	1.89	0.54
1:J:130:ASP:HA	1:J:133:HIS:HB3	1.89	0.54
1:L:177:GLN:O	1:L:269:VAL:HG22	2.07	0.54
1:E:30:GLN:HG2	1:E:107:TYR:CD2	2.42	0.54
1:C:20:GLY:O	1:C:23:THR:HG22	2.07	0.54
1:C:321:LEU:C	1:C:323:GLY:H	2.10	0.54
1:E:186:ARG:NH2	1:F:18:LEU:HD21	2.23	0.54
1:E:417:LEU:HB2	1:F:116:ILE:HD13	1.89	0.54
1:G:248:ALA:HA	1:G:283:GLN:HE22	1.71	0.54
1:E:400:LEU:HD21	1:E:457:LEU:HB3	1.90	0.54
1:J:214:LEU:HD11	1:J:259:LEU:HD22	1.90	0.54
1:H:320:SER:O	1:H:323:GLY:N	2.36	0.54
1:I:180:ARG:HD2	1:I:206:ILE:HD11	1.89	0.54
1:A:80:MET:HE1	1:A:89:TRP:CH2	2.43	0.54
1:B:36:ASP:OD2	1:F:109:ARG:HD3	2.08	0.54
1:D:61:THR:HG21	1:D:91:ARG:HE	1.72	0.54
1:D:147:VAL:CG1	1:D:156:VAL:HG23	2.38	0.54
1:D:83:PHE:HA	1:D:129:GLY:HA2	1.90	0.54
1:E:96:ASN:OD1	1:E:97:LYS:N	2.41	0.54
1:J:310:LEU:HD22	1:J:391:ILE:HG13	1.90	0.54
1:C:284:LEU:HD12	1:C:285:PRO:HD2	1.89	0.54
1:I:192:GLU:OE1	1:I:195:LYS:NZ	2.41	0.54
1:J:476:ASP:O	1:J:480:PHE:N	2.41	0.54
1:L:151:TRP:O	1:L:157:ARG:NE	2.39	0.54
1:B:31:ALA:O	1:B:34:ILE:HB	2.08	0.53
1:I:112:PRO:O	1:I:116:ILE:HG23	2.08	0.53
1:L:340:GLU:O	1:L:340:GLU:HG2	2.08	0.53
1:L:429:ASP:OD1	1:L:430:PHE:N	2.40	0.53
1:A:165:ARG:NH2	1:A:320:SER:HB2	2.23	0.53
1:E:8:GLU:OE1	1:E:49:VAL:HG21	2.07	0.53
1:F:417:LEU:HD23	1:F:421:ARG:HE	1.74	0.53
1:G:311:VAL:O	1:G:315:LYS:HB2	2.09	0.53
1:H:343:LEU:HD11	1:H:421:ARG:HB2	1.90	0.53
1:J:12:LEU:HD11	1:J:63:ILE:HG21	1.89	0.53
1:C:432:ARG:O	1:C:435:THR:HG22	2.08	0.53
1:H:150:HIS:CE1	1:H:152:GLU:HG3	2.44	0.53
1:B:7:TYR:O	1:B:46:SER:HB3	2.08	0.53
1:B:298:GLY:HA2	1:B:311:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:482:LYS:HB3	1:E:486:TRP:CH2	2.44	0.53
1:A:108:ASN:ND2	1:A:120:TYR:OH	2.34	0.53
1:G:328:MET:HB2	1:G:448:PHE:HB2	1.91	0.53
1:H:145:LYS:HD2	1:H:459:ASP:OD1	2.09	0.53
1:J:239:MET:HG3	1:J:361:ILE:HG22	1.90	0.53
1:B:315:LYS:HD2	1:B:325:THR:HB	1.90	0.53
1:G:417:LEU:HD23	1:G:421:ARG:HE	1.74	0.53
1:I:215:ALA:O	1:I:218:VAL:HG22	2.09	0.53
1:K:107:TYR:HA	1:K:151:TRP:HE1	1.74	0.53
1:B:397:ARG:HH22	1:B:399:ARG:HH21	1.56	0.53
1:D:493:LEU:HG	1:D:494:LEU:H	1.73	0.53
1:F:488:GLU:OE2	1:G:141:ARG:NH1	2.41	0.53
1:G:340:GLU:HG3	1:G:430:PHE:HB3	1.91	0.53
1:L:278:LEU:HD13	1:L:284:LEU:HA	1.90	0.53
1:L:458:ILE:HD11	1:L:470:VAL:HG11	1.90	0.53
1:E:86:SER:OG	1:E:132:GLU:OE2	2.27	0.53
1:G:11:PHE:O	1:G:12:LEU:HD12	2.09	0.53
1:I:417:LEU:HB3	1:I:421:ARG:HH21	1.74	0.53
1:J:269:VAL:HB	1:J:312:ARG:HG2	1.90	0.53
1:A:224:ARG:HA	1:A:227:GLU:HG2	1.91	0.52
1:J:92:GLY:O	1:J:95:ILE:HG22	2.09	0.52
1:A:344:GLY:HA3	1:A:424:TRP:CZ3	2.44	0.52
1:B:140:MET:HB3	1:B:142:LEU:HD23	1.90	0.52
1:D:7:TYR:CD2	1:D:168:CYS:HB2	2.44	0.52
1:I:48:ILE:HD11	1:I:164:MET:HE1	1.92	0.52
1:K:54:LEU:HD21	1:K:63:ILE:HG13	1.91	0.52
1:K:293:MET:O	1:K:315:LYS:NZ	2.42	0.52
1:L:169:ALA:HA	1:L:316:VAL:HG11	1.91	0.52
1:H:41:ASP:OD1	1:H:43:ILE:HG22	2.10	0.52
1:A:343:LEU:HD11	1:A:421:ARG:HB2	1.91	0.52
1:C:130:ASP:HA	1:C:133:HIS:HB3	1.91	0.52
1:H:313:ALA:O	1:H:317:MET:HG3	2.10	0.52
1:J:86:SER:OG	1:J:133:HIS:HA	2.10	0.52
1:L:140:MET:HB3	1:L:142:LEU:HD23	1.90	0.52
1:A:284:LEU:HD12	1:A:285:PRO:HD2	1.92	0.52
1:B:403:ASN:HA	1:B:471:ILE:HB	1.91	0.52
1:C:314:ILE:HD11	1:C:452:ILE:HD11	1.91	0.52
1:E:35:VAL:HG21	1:E:50:LEU:HB2	1.92	0.52
1:G:329:GLU:OE1	1:G:346:HIS:NE2	2.42	0.52
1:I:96:ASN:ND2	1:I:100:LEU:HD21	2.24	0.52
1:K:130:ASP:HA	1:K:133:HIS:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LYS:HE2	1:B:163:TRP:HB2	1.91	0.52
1:E:322:PRO:O	1:E:323:GLY:O	2.28	0.52
1:I:102:HIS:NE2	1:I:130:ASP:HB2	2.24	0.52
1:I:232:GLU:O	1:I:235:GLU:HB2	2.10	0.52
1:C:101:LEU:HD13	1:C:160:ILE:HG13	1.91	0.52
1:C:403:ASN:HA	1:C:471:ILE:HB	1.90	0.52
1:D:403:ASN:HD21	1:D:433:ALA:HB1	1.75	0.52
1:E:4:LEU:HD11	1:E:45:PRO:HB2	1.92	0.52
1:G:180:ARG:HD2	1:G:206:ILE:HD11	1.91	0.52
1:J:405:VAL:HG12	1:J:426:PRO:HA	1.91	0.52
1:L:214:LEU:HD23	1:L:281:LEU:HD11	1.91	0.52
1:C:304:ASP:OD2	1:C:445:HIS:HB2	2.10	0.52
1:C:313:ALA:O	1:C:317:MET:HG3	2.09	0.52
1:L:284:LEU:HD12	1:L:285:PRO:HD2	1.91	0.52
1:D:116:ILE:HG22	1:D:120:TYR:CE2	2.45	0.52
1:E:458:ILE:O	1:E:462:GLU:HB2	2.10	0.52
1:I:184:ASN:ND2	1:I:192:GLU:OE2	2.42	0.52
1:A:8:GLU:O	1:A:73:CYS:HA	2.11	0.51
1:E:485:ARG:HB2	1:F:490:TYR:CD2	2.45	0.51
1:F:284:LEU:HD23	1:F:374:PRO:HG3	1.92	0.51
1:H:107:TYR:HE1	1:H:124:ASN:HD21	1.57	0.51
1:J:237:TYR:HA	1:J:358:LYS:HE2	1.92	0.51
1:F:322:PRO:O	1:F:323:GLY:O	2.28	0.51
1:H:284:LEU:HD12	1:H:285:PRO:HD2	1.92	0.51
1:J:172:ASP:OD2	1:J:312:ARG:NH2	2.42	0.51
1:J:432:ARG:O	1:J:435:THR:HG22	2.10	0.51
1:K:222:PRO:HB2	1:K:225:GLU:HG3	1.92	0.51
1:A:79:TRP:NE1	1:A:105:THR:O	2.44	0.51
1:C:180:ARG:HG2	1:C:272:THR:CG2	2.40	0.51
1:C:482:LYS:HB3	1:C:486:TRP:CZ2	2.45	0.51
1:E:39:ASN:ND2	1:E:48:ILE:HB	2.25	0.51
1:E:485:ARG:HB2	1:F:490:TYR:CD1	2.46	0.51
1:F:248:ALA:HA	1:F:283:GLN:HE22	1.75	0.51
1:H:30:GLN:HE22	1:H:123:LEU:HD21	1.74	0.51
1:K:310:LEU:HD22	1:K:391:ILE:HG13	1.91	0.51
1:B:30:GLN:HG2	1:B:107:TYR:CD2	2.46	0.51
1:G:209:TRP:CZ2	1:G:266:LYS:HG2	2.45	0.51
1:K:140:MET:HB3	1:K:142:LEU:HD23	1.92	0.51
1:K:310:LEU:HD13	1:K:391:ILE:HD11	1.93	0.51
1:K:431:LYS:O	1:K:435:THR:HG22	2.10	0.51
1:B:312:ARG:O	1:B:316:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:ASN:ND2	1:H:120:TYR:OH	2.36	0.51
1:I:70:ASP:OD1	1:I:72:LYS:N	2.43	0.51
1:J:311:VAL:O	1:J:315:LYS:HB2	2.10	0.51
1:L:166:VAL:HG21	1:L:459:ASP:HB2	1.93	0.51
1:L:191:THR:HA	1:L:304:ASP:OD2	2.11	0.51
1:D:191:THR:HG22	1:D:304:ASP:HB2	1.92	0.51
1:F:153:GLU:OE2	1:F:155:GLU:HB3	2.11	0.51
1:H:279:HIS:NE2	1:K:213:GLU:HG2	2.26	0.51
1:B:199:GLN:HG2	1:B:204:TRP:O	2.10	0.51
1:E:435:THR:CG2	1:E:477:LEU:HD21	2.40	0.51
1:F:418:PRO:HG3	1:G:118:MET:HG2	1.92	0.51
1:G:428:PRO:HG2	1:G:432:ARG:HH11	1.75	0.51
1:B:269:VAL:HB	1:B:312:ARG:HG2	1.92	0.51
1:C:17:TYR:O	1:C:19:TYR:N	2.43	0.51
1:D:215:ALA:HB1	1:D:280:ASP:HB3	1.93	0.51
1:D:329:GLU:OE1	1:D:445:HIS:CE1	2.64	0.51
1:H:183:ASP:OD2	1:K:180:ARG:NH1	2.44	0.51
1:K:80:MET:CG	1:K:130:ASP:HB3	2.40	0.51
1:E:314:ILE:HG23	1:E:325:THR:HG21	1.92	0.50
1:E:340:GLU:HG3	1:E:430:PHE:HB3	1.93	0.50
1:G:50:LEU:C	1:G:50:LEU:HD23	2.31	0.50
1:H:362:GLU:HB3	1:H:364:HIS:HE2	1.76	0.50
1:I:298:GLY:HA2	1:I:311:VAL:HG12	1.92	0.50
1:L:458:ILE:O	1:L:462:GLU:HB2	2.11	0.50
1:C:156:VAL:O	1:C:160:ILE:HG22	2.11	0.50
1:F:363:VAL:HG12	1:F:375:ALA:HA	1.92	0.50
1:A:91:ARG:NH2	4:A:601:HOH:O	2.41	0.50
1:C:107:TYR:CE2	1:C:124:ASN:ND2	2.77	0.50
1:D:30:GLN:HG2	1:D:107:TYR:CD2	2.46	0.50
1:E:101:LEU:HA	1:E:145:LYS:O	2.11	0.50
1:F:346:HIS:O	1:F:419:THR:HG21	2.10	0.50
1:I:195:LYS:HG3	1:I:206:ILE:HD13	1.94	0.50
1:K:20:GLY:O	1:K:23:THR:HG22	2.12	0.50
1:A:201:LYS:CE	1:A:465:GLU:O	2.60	0.50
1:B:392:VAL:HG11	1:B:441:GLY:O	2.11	0.50
1:C:28:GLU:HG2	1:C:53:VAL:HG23	1.93	0.50
1:H:4:LEU:HD11	1:H:45:PRO:HB2	1.94	0.50
1:F:199:GLN:HG2	1:F:204:TRP:O	2.11	0.50
1:H:60:ILE:HG21	1:H:89:TRP:HA	1.94	0.50
1:K:218:VAL:O	1:K:254:LYS:HD3	2.11	0.50
1:A:112:PRO:HB2	1:A:115:THR:HB	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:283:GLN:OE1	1:F:374:PRO:HA	2.12	0.49
1:G:179:VAL:O	1:G:271:PHE:HA	2.12	0.49
1:I:269:VAL:HB	1:I:312:ARG:HG2	1.94	0.49
1:B:378:VAL:HG22	1:B:418:PRO:O	2.12	0.49
1:G:314:ILE:HD11	1:G:452:ILE:HD11	1.93	0.49
1:H:112:PRO:HB2	1:H:115:THR:HB	1.94	0.49
1:H:262:PHE:CD1	1:H:266:LYS:HG3	2.47	0.49
1:L:3:ASP:OD1	1:L:3:ASP:C	2.51	0.49
1:L:343:LEU:HD11	1:L:421:ARG:HB2	1.93	0.49
1:J:320:SER:O	1:J:323:GLY:N	2.44	0.49
1:L:403:ASN:HA	1:L:471:ILE:HB	1.94	0.49
1:B:107:TYR:CE2	1:B:124:ASN:OD1	2.66	0.49
1:B:380:ASP:HB3	1:B:410:ILE:HD13	1.94	0.49
1:F:195:LYS:HG3	1:F:206:ILE:HD13	1.95	0.49
1:F:410:ILE:HG13	1:F:423:LEU:HD12	1.93	0.49
1:G:321:LEU:C	1:G:323:GLY:H	2.16	0.49
1:H:432:ARG:O	1:H:435:THR:HG22	2.12	0.49
1:C:50:LEU:HD23	1:C:51:LYS:N	2.27	0.49
1:C:211:VAL:HG11	1:C:278:LEU:HA	1.93	0.49
1:D:251:GLU:O	1:D:254:LYS:HG2	2.12	0.49
1:H:30:GLN:HG2	1:H:107:TYR:CE2	2.48	0.49
1:J:314:ILE:HG23	1:J:325:THR:HG21	1.93	0.49
1:J:490:TYR:CG	1:K:485:ARG:HB2	2.47	0.49
1:A:120:TYR:CG	1:A:120:TYR:O	2.65	0.49
1:A:467:GLU:HB2	1:A:491:TRP:CD1	2.48	0.49
1:B:55:LYS:O	1:B:88:MET:SD	2.71	0.49
1:E:114:ASP:HA	1:G:415:PRO:HD2	1.94	0.49
1:E:343:LEU:HD11	1:E:421:ARG:HB2	1.93	0.49
1:F:284:LEU:HD12	1:F:285:PRO:HD2	1.95	0.49
1:K:343:LEU:HD11	1:K:421:ARG:HB2	1.93	0.49
1:A:478:GLU:OE1	1:D:458:ILE:HD13	2.12	0.49
1:C:4:LEU:HD11	1:C:45:PRO:HB2	1.94	0.49
1:L:201:LYS:NZ	1:L:495:LYS:HG2	2.28	0.49
1:L:493:LEU:HD23	1:L:493:LEU:H	1.77	0.49
1:B:7:TYR:CD2	1:B:168:CYS:HB2	2.47	0.49
1:D:21:LEU:HD12	1:D:24:LEU:HD12	1.95	0.49
1:E:162:LYS:CD	1:E:455:GLU:HG2	2.42	0.49
1:E:493:LEU:HG	1:E:494:LEU:H	1.77	0.49
1:L:54:LEU:HB3	1:L:60:ILE:HD13	1.94	0.49
1:A:141:ARG:HH22	1:C:394:MET:HB3	1.78	0.49
1:A:222:PRO:CG	1:H:22:GLU:HG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LEU:HD12	1:C:263:LEU:HD11	1.94	0.49
1:H:180:ARG:HB2	1:H:208:THR:HG23	1.94	0.49
1:I:162:LYS:CD	1:I:455:GLU:HG2	2.38	0.49
1:C:135:PHE:HA	1:D:441:GLY:CA	2.43	0.49
1:J:180:ARG:HG2	1:J:272:THR:CG2	2.43	0.49
1:K:35:VAL:HG21	1:K:50:LEU:HB2	1.94	0.49
1:K:328:MET:HB2	1:K:448:PHE:HB2	1.95	0.49
1:K:140:MET:CB	1:K:142:LEU:HD23	2.43	0.48
1:A:84:SER:O	1:A:84:SER:OG	2.30	0.48
1:A:106:GLN:NE2	1:C:332:THR:OG1	2.45	0.48
1:C:10:TRP:CE3	1:C:51:LYS:HD2	2.47	0.48
1:D:116:ILE:HG22	1:D:120:TYR:CD2	2.48	0.48
1:E:153:GLU:OE2	1:G:431:LYS:HE2	2.13	0.48
1:F:202:LEU:HD22	1:F:464:LEU:HD13	1.94	0.48
1:A:56:SER:HB3	1:A:59:GLU:HG3	1.94	0.48
1:A:135:PHE:CE1	1:C:392:VAL:HG22	2.47	0.48
1:A:178:ILE:HA	1:A:270:GLY:O	2.13	0.48
1:B:215:ALA:O	1:B:218:VAL:HG22	2.14	0.48
1:C:184:ASN:ND2	1:C:192:GLU:HA	2.28	0.48
1:H:361:ILE:HA	1:H:376:ARG:O	2.14	0.48
1:H:363:VAL:O	1:H:363:VAL:HG23	2.12	0.48
1:I:214:LEU:HD21	1:I:259:LEU:HD21	1.94	0.48
1:A:183:ASP:OD2	1:F:180:ARG:NH1	2.46	0.48
1:A:271:PHE:O	1:A:299:PHE:HA	2.13	0.48
1:C:17:TYR:C	1:C:19:TYR:H	2.17	0.48
1:K:293:MET:SD	1:K:299:PHE:HB3	2.53	0.48
1:L:314:ILE:HG23	1:L:325:THR:HG21	1.95	0.48
1:A:41:ASP:OD1	1:A:43:ILE:HG22	2.14	0.48
1:A:132:GLU:OE2	1:C:189:ALA:N	2.41	0.48
1:B:223:GLU:O	1:B:226:VAL:HG22	2.13	0.48
1:C:87:LYS:HB2	1:D:187:GLU:HA	1.95	0.48
1:C:162:LYS:HD2	1:C:455:GLU:HG2	1.95	0.48
1:K:242:ASP:HA	1:K:246:LEU:HD22	1.95	0.48
1:L:320:SER:OG	1:L:322:PRO:HD2	2.12	0.48
1:B:321:LEU:C	1:B:323:GLY:H	2.16	0.48
1:E:135:PHE:CD1	1:G:392:VAL:HG21	2.48	0.48
1:E:315:LYS:HD2	1:E:325:THR:HB	1.95	0.48
1:E:403:ASN:HD21	1:E:426:PRO:HB3	1.78	0.48
1:I:396:ASN:OD1	1:I:397:ARG:N	2.47	0.48
1:J:128:HIS:HB2	1:K:444:HIS:HB2	1.96	0.48
1:K:314:ILE:HD11	1:K:452:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ASP:OD1	1:A:307:ALA:N	2.40	0.48
1:B:312:ARG:O	1:B:312:ARG:HD2	2.14	0.48
1:D:100:LEU:O	1:D:144:ARG:HB2	2.14	0.48
1:E:278:LEU:O	1:E:371:LYS:NZ	2.46	0.48
1:E:403:ASN:O	1:E:405:VAL:HG13	2.13	0.48
1:L:143:PRO:HG3	1:L:465:GLU:CD	2.34	0.48
1:L:233:TYR:O	1:L:237:TYR:N	2.39	0.48
1:A:150:HIS:CE1	1:A:152:GLU:HG3	2.48	0.48
1:B:78:VAL:HG11	1:B:133:HIS:CE1	2.49	0.48
1:E:332:THR:HG22	1:E:343:LEU:HB3	1.95	0.48
1:F:225:GLU:O	1:F:228:GLU:N	2.46	0.48
1:F:399:ARG:NH1	1:F:440:ALA:O	2.44	0.48
1:G:325:THR:HA	1:G:449:SER:HA	1.94	0.48
1:G:435:THR:HG23	1:G:477:LEU:HD21	1.96	0.48
1:J:343:LEU:HD11	1:J:421:ARG:HB2	1.94	0.48
1:B:278:LEU:HD13	1:B:284:LEU:HA	1.96	0.48
1:F:92:GLY:O	1:F:95:ILE:HG22	2.14	0.48
1:K:467:GLU:HA	1:K:491:TRP:CE2	2.49	0.48
1:L:269:VAL:HB	1:L:312:ARG:HG2	1.96	0.48
1:A:26:LYS:HD2	1:H:225:GLU:OE2	2.14	0.48
1:B:107:TYR:CZ	1:B:108:ASN:ND2	2.82	0.48
1:C:162:LYS:O	1:C:166:VAL:HG23	2.14	0.48
1:D:80:MET:HG3	1:D:130:ASP:HB3	1.96	0.48
1:E:485:ARG:HD2	1:F:490:TYR:CE2	2.49	0.48
1:A:26:LYS:O	1:A:30:GLN:HG3	2.14	0.47
1:E:116:ILE:O	1:E:116:ILE:CD1	2.62	0.47
1:E:116:ILE:HD11	1:G:414:MET:HB3	1.96	0.47
1:G:135:PHE:O	1:G:139:ARG:N	2.35	0.47
1:G:165:ARG:NH2	1:G:320:SER:OG	2.47	0.47
1:I:482:LYS:HB3	1:I:486:TRP:CH2	2.49	0.47
1:L:172:ASP:OD2	1:L:312:ARG:NE	2.46	0.47
1:A:218:VAL:O	1:A:254:LYS:HD2	2.14	0.47
1:E:8:GLU:O	1:E:73:CYS:HA	2.13	0.47
1:E:135:PHE:CE1	1:G:392:VAL:HG22	2.49	0.47
1:F:80:MET:HG3	1:F:130:ASP:HA	1.95	0.47
1:F:107:TYR:HA	1:F:151:TRP:HE1	1.80	0.47
1:J:278:LEU:HD13	1:J:284:LEU:HA	1.95	0.47
1:A:107:TYR:HA	1:A:151:TRP:HE1	1.79	0.47
1:A:223:GLU:O	1:A:226:VAL:HG22	2.14	0.47
1:B:60:ILE:HG22	1:B:92:GLY:HA3	1.96	0.47
1:C:314:ILE:HD12	1:C:457:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:LEU:HD11	1:D:421:ARG:HB2	1.96	0.47
1:D:426:PRO:HB2	1:D:433:ALA:HB3	1.97	0.47
1:E:489:LEU:HD13	1:F:489:LEU:HB2	1.95	0.47
1:F:290:GLN:HE22	1:F:377:LEU:H	1.61	0.47
1:I:314:ILE:HG23	1:I:325:THR:HG21	1.96	0.47
1:A:123:LEU:HD23	1:A:124:ASN:N	2.30	0.47
1:C:142:LEU:HD13	1:C:143:PRO:HD2	1.96	0.47
1:D:453:ASP:OD1	1:D:454:VAL:N	2.48	0.47
1:G:320:SER:HB3	1:G:322:PRO:HD2	1.96	0.47
1:H:3:ASP:C	1:H:3:ASP:OD1	2.52	0.47
1:J:106:GLN:HE21	1:J:126:SER:HB3	1.80	0.47
1:A:187:GLU:O	1:D:87:LYS:HB2	2.14	0.47
1:A:199:GLN:HG2	1:A:204:TRP:O	2.14	0.47
1:A:394:MET:HE3	1:D:139:ARG:HA	1.97	0.47
1:C:116:ILE:HD11	1:D:414:MET:HB3	1.96	0.47
1:D:190:SER:O	1:D:306:LYS:NZ	2.47	0.47
1:G:15:SER:HA	1:G:82:THR:HG23	1.96	0.47
1:G:278:LEU:HD13	1:G:284:LEU:HA	1.97	0.47
1:I:475:LEU:HD11	1:I:477:LEU:HD23	1.96	0.47
1:J:21:LEU:HD12	1:J:24:LEU:HD12	1.97	0.47
1:A:35:VAL:HG21	1:A:50:LEU:HB2	1.97	0.47
1:C:397:ARG:HH22	1:C:399:ARG:HH21	1.62	0.47
1:D:304:ASP:OD1	1:D:307:ALA:CB	2.62	0.47
1:E:80:MET:HE1	1:E:89:TRP:CZ2	2.50	0.47
1:E:134:GLY:HA3	1:G:438:ILE:HG23	1.97	0.47
1:I:183:ASP:OD2	1:J:180:ARG:NH1	2.48	0.47
1:A:184:ASN:ND2	1:A:192:GLU:OE2	2.48	0.47
1:A:185:MET:HB2	1:A:302:GLU:HB3	1.96	0.47
1:A:417:LEU:HD12	1:A:418:PRO:HD2	1.97	0.47
1:A:431:LYS:O	1:A:435:THR:HB	2.14	0.47
1:B:314:ILE:HG23	1:B:325:THR:HG21	1.95	0.47
1:C:346:HIS:O	1:C:419:THR:HG21	2.15	0.47
1:C:364:HIS:HB2	1:C:376:ARG:NH2	2.29	0.47
1:D:292:LEU:O	1:D:295:GLU:HB2	2.14	0.47
1:E:136:ILE:HG13	1:E:140:MET:SD	2.55	0.47
1:F:313:ALA:O	1:F:317:MET:HG3	2.14	0.47
1:G:315:LYS:HD2	1:G:325:THR:HB	1.96	0.47
1:I:104:HIS:CD2	1:I:148:VAL:HG13	2.49	0.47
1:I:223:GLU:O	1:I:226:VAL:HG22	2.15	0.47
1:K:34:ILE:O	1:K:38:LEU:HD13	2.15	0.47
1:K:74:ALA:HB1	1:K:168:CYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:223:GLU:O	1:K:226:VAL:HG22	2.15	0.47
1:A:184:ASN:ND2	1:A:192:GLU:CD	2.68	0.47
1:C:41:ASP:CG	1:C:43:ILE:HG22	2.36	0.47
1:E:54:LEU:HD21	1:E:63:ILE:HG13	1.96	0.47
1:F:185:MET:HB2	1:F:302:GLU:HB3	1.97	0.47
1:F:215:ALA:HA	1:F:218:VAL:HG22	1.96	0.47
1:G:55:LYS:O	1:G:88:MET:SD	2.73	0.47
1:G:140:MET:HB3	1:G:142:LEU:HD23	1.97	0.47
1:G:321:LEU:C	1:G:323:GLY:N	2.68	0.47
1:H:41:ASP:OD2	1:H:157:ARG:NH1	2.48	0.47
1:J:102:HIS:NE2	1:J:130:ASP:HB2	2.30	0.47
1:K:310:LEU:HB2	1:K:391:ILE:HD12	1.97	0.47
1:E:180:ARG:HG2	1:E:272:THR:CG2	2.45	0.47
1:E:186:ARG:CZ	1:F:18:LEU:HD21	2.45	0.47
1:F:107:TYR:CD1	1:F:108:ASN:N	2.83	0.47
1:H:121:MET:HE1	1:I:343:LEU:HD23	1.97	0.47
1:J:107:TYR:HA	1:J:151:TRP:HE1	1.80	0.47
1:J:403:ASN:O	1:J:405:VAL:HG13	2.13	0.47
1:C:186:ARG:HG2	1:G:207:ASN:HB3	1.96	0.47
1:G:444:HIS:O	1:G:446:THR:HG23	2.15	0.47
1:I:179:VAL:O	1:I:271:PHE:HA	2.15	0.47
1:I:214:LEU:HD11	1:I:259:LEU:HD22	1.96	0.47
1:J:51:LYS:HB3	1:J:52:PRO:HD2	1.97	0.47
1:B:54:LEU:HD22	1:B:59:GLU:HB3	1.96	0.46
1:C:96:ASN:HD21	1:C:100:LEU:HD23	1.81	0.46
1:D:19:TYR:HB3	1:D:23:THR:CG2	2.44	0.46
1:E:156:VAL:O	1:E:160:ILE:HG22	2.15	0.46
1:F:101:LEU:HD13	1:F:160:ILE:HG13	1.97	0.46
1:I:54:LEU:HD13	1:I:60:ILE:HA	1.97	0.46
1:J:143:PRO:HB3	1:J:465:GLU:CG	2.45	0.46
1:A:333:TYR:H	1:D:106:GLN:HE22	1.63	0.46
1:C:2:ILE:HD12	1:C:312:ARG:HH12	1.80	0.46
1:C:410:ILE:HG13	1:C:423:LEU:HD12	1.97	0.46
1:E:444:HIS:ND1	1:F:132:GLU:HB2	2.30	0.46
1:H:116:ILE:HG22	1:H:120:TYR:CE2	2.50	0.46
1:I:493:LEU:HD23	1:I:493:LEU:H	1.80	0.46
1:J:139:ARG:NH1	1:K:395:GLY:HA2	2.29	0.46
1:L:180:ARG:HD2	1:L:206:ILE:HD11	1.97	0.46
1:A:7:TYR:CD2	1:A:168:CYS:HB2	2.51	0.46
1:F:239:MET:SD	1:F:245:SER:HB3	2.54	0.46
1:J:68:ASN:HD21	1:J:97:LYS:H	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:112:PRO:HB2	1:J:115:THR:HB	1.97	0.46
1:H:54:LEU:HD21	1:H:63:ILE:HG13	1.97	0.46
1:K:401:VAL:HA	1:K:469:VAL:HG23	1.97	0.46
1:L:211:VAL:HG21	1:L:277:ASP:O	2.15	0.46
1:B:67:ALA:O	1:B:98:LYS:NZ	2.38	0.46
1:B:307:ALA:O	1:B:310:LEU:HB3	2.16	0.46
1:C:232:GLU:O	1:C:232:GLU:HG2	2.16	0.46
1:C:330:ASP:OD1	1:C:330:ASP:N	2.45	0.46
1:G:270:GLY:HA2	1:G:298:GLY:O	2.15	0.46
1:H:315:LYS:HD2	1:H:325:THR:HB	1.97	0.46
1:H:362:GLU:HB3	1:H:364:HIS:NE2	2.30	0.46
1:I:4:LEU:HD11	1:I:45:PRO:HB2	1.97	0.46
1:I:13:VAL:HB	1:I:53:VAL:HG22	1.98	0.46
1:A:56:SER:O	1:A:60:ILE:HG12	2.16	0.46
1:C:184:ASN:OD1	1:C:184:ASN:N	2.48	0.46
1:D:214:LEU:HD23	1:D:281:LEU:HD11	1.98	0.46
1:E:394:MET:O	1:E:396:ASN:N	2.49	0.46
1:F:180:ARG:HD2	1:F:206:ILE:HD11	1.98	0.46
1:G:80:MET:SD	1:G:84:SER:OG	2.61	0.46
1:H:55:LYS:O	1:H:88:MET:SD	2.73	0.46
1:J:490:TYR:CD2	1:K:485:ARG:HB2	2.50	0.46
1:A:13:VAL:HB	1:A:53:VAL:HG22	1.97	0.46
1:A:493:LEU:H	1:A:493:LEU:HD23	1.80	0.46
1:C:141:ARG:HH22	1:D:394:MET:HB3	1.81	0.46
1:C:298:GLY:HA2	1:C:311:VAL:HG12	1.98	0.46
1:G:74:ALA:HB1	1:G:168:CYS:HA	1.97	0.46
1:G:104:HIS:CE1	1:G:130:ASP:OD1	2.68	0.46
1:H:104:HIS:CD2	1:H:148:VAL:HG13	2.51	0.46
1:I:145:LYS:HE2	1:I:163:TRP:HB2	1.98	0.46
1:J:86:SER:O	1:J:87:LYS:C	2.54	0.46
1:J:284:LEU:HD23	1:J:374:PRO:HG3	1.97	0.46
1:K:397:ARG:NH1	1:K:467:GLU:OE1	2.37	0.46
1:L:397:ARG:HH22	1:L:399:ARG:HH21	1.64	0.46
1:A:32:SER:O	1:A:36:ASP:HB2	2.16	0.46
1:A:111:ILE:HG22	1:A:116:ILE:HG12	1.98	0.46
1:A:240:PRO:O	1:A:246:LEU:HB2	2.16	0.46
1:B:315:LYS:CD	1:B:325:THR:HB	2.46	0.46
1:C:311:VAL:O	1:C:315:LYS:HB2	2.16	0.46
1:E:290:GLN:NE2	1:E:348:LEU:O	2.49	0.46
1:G:284:LEU:HD12	1:G:285:PRO:HD2	1.97	0.46
1:G:493:LEU:HG	1:G:494:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:133:HIS:O	1:I:133:HIS:CG	2.69	0.46
1:K:246:LEU:HA	1:K:249:ILE:HG12	1.97	0.46
1:L:273:THR:HG21	1:L:285:PRO:HG2	1.98	0.46
1:D:332:THR:O	1:D:343:LEU:N	2.48	0.46
1:E:100:LEU:HB3	1:E:144:ARG:HB2	1.97	0.46
1:E:311:VAL:O	1:E:315:LYS:HB2	2.16	0.46
1:F:223:GLU:O	1:F:226:VAL:HG22	2.16	0.46
1:G:162:LYS:O	1:G:166:VAL:HG23	2.16	0.46
1:I:266:LYS:O	1:I:267:ASN:C	2.53	0.46
1:K:278:LEU:HD13	1:K:284:LEU:HA	1.97	0.46
1:L:34:ILE:O	1:L:38:LEU:HB2	2.16	0.46
1:B:245:SER:HA	1:B:363:VAL:HG21	1.98	0.46
1:C:172:ASP:CG	1:C:172:ASP:O	2.55	0.46
1:A:426:PRO:HB2	1:A:433:ALA:HB3	1.98	0.45
1:C:51:LYS:HB3	1:C:52:PRO:HD2	1.98	0.45
1:D:397:ARG:NH1	1:D:467:GLU:OE1	2.47	0.45
1:I:328:MET:HB2	1:I:448:PHE:HB2	1.98	0.45
1:I:381:GLY:HA3	1:I:422:VAL:HG13	1.97	0.45
1:J:11:PHE:HB3	1:J:50:LEU:HA	1.96	0.45
1:C:269:VAL:HB	1:C:312:ARG:HG2	1.96	0.45
1:D:321:LEU:C	1:D:323:GLY:H	2.20	0.45
1:D:443:SER:HB3	1:D:445:HIS:O	2.16	0.45
1:E:3:ASP:OD2	1:E:5:LYS:HE2	2.16	0.45
1:H:340:GLU:H	1:H:340:GLU:CD	2.19	0.45
1:J:10:TRP:CE3	1:J:51:LYS:HD2	2.51	0.45
1:J:389:ALA:O	1:J:447:ALA:N	2.44	0.45
1:A:47:LYS:O	1:A:48:ILE:HG13	2.16	0.45
1:B:30:GLN:O	1:B:34:ILE:HG13	2.16	0.45
1:D:3:ASP:C	1:D:3:ASP:OD1	2.53	0.45
1:D:376:ARG:HH11	1:D:418:PRO:HB2	1.81	0.45
1:G:214:LEU:HD11	1:G:259:LEU:HD22	1.97	0.45
1:H:31:ALA:HB1	1:H:50:LEU:HD11	1.99	0.45
1:J:101:LEU:HB2	1:J:163:TRP:CD2	2.51	0.45
1:J:180:ARG:HA	1:J:272:THR:HG23	1.98	0.45
1:J:311:VAL:HG21	1:J:327:PHE:HB2	1.99	0.45
1:A:263:LEU:HB3	1:A:268:ALA:HB3	1.99	0.45
1:C:184:ASN:HD21	1:C:192:GLU:HA	1.81	0.45
1:G:10:TRP:CE3	1:G:51:LYS:HD2	2.51	0.45
1:K:429:ASP:HB3	1:K:432:ARG:HG3	1.98	0.45
1:B:186:ARG:NH1	1:B:276:GLU:HG3	2.32	0.45
1:E:96:ASN:OD1	1:E:96:ASN:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:141:ARG:HH22	1:I:394:MET:HB3	1.81	0.45
1:H:311:VAL:O	1:H:315:LYS:HB2	2.16	0.45
1:I:17:TYR:N	1:I:55:LYS:HB2	2.31	0.45
1:J:390:SER:HB2	1:J:446:THR:HA	1.97	0.45
1:A:402:VAL:HG21	1:A:457:LEU:HD12	1.98	0.45
1:C:252:GLN:HG3	1:C:375:ALA:HB3	1.98	0.45
1:D:160:ILE:O	1:D:164:MET:HG3	2.16	0.45
1:E:12:LEU:HD22	1:E:76:VAL:HG11	1.98	0.45
1:G:403:ASN:HA	1:G:471:ILE:HB	1.98	0.45
1:H:177:GLN:OE1	1:H:207:ASN:ND2	2.47	0.45
1:H:316:VAL:O	1:H:319:THR:OG1	2.35	0.45
1:J:141:ARG:HH22	1:K:394:MET:HB3	1.82	0.45
1:L:41:ASP:OD1	1:L:43:ILE:HG22	2.15	0.45
1:A:54:LEU:HD21	1:A:63:ILE:HG13	1.99	0.45
1:A:362:GLU:HB3	1:A:364:HIS:CD2	2.52	0.45
1:D:4:LEU:CD1	1:D:45:PRO:HB2	2.46	0.45
1:F:428:PRO:HG3	1:F:473:GLU:O	2.17	0.45
1:I:340:GLU:HG3	1:I:430:PHE:HB3	1.99	0.45
1:J:116:ILE:HG22	1:J:120:TYR:CE2	2.52	0.45
1:K:179:VAL:O	1:K:271:PHE:HA	2.16	0.45
1:L:102:HIS:NE2	1:L:130:ASP:HB2	2.32	0.45
1:A:293:MET:O	1:A:296:GLY:N	2.50	0.45
1:B:399:ARG:NH1	1:B:484:LEU:HD22	2.32	0.45
1:C:80:MET:HE1	1:C:89:TRP:CZ2	2.51	0.45
1:E:429:ASP:OD1	1:E:430:PHE:N	2.49	0.45
1:J:64:PHE:O	1:J:67:ALA:N	2.48	0.45
1:A:80:MET:CG	1:A:130:ASP:HB3	2.47	0.45
1:A:315:LYS:HD2	1:A:325:THR:HB	1.99	0.45
1:A:403:ASN:HA	1:A:471:ILE:HB	1.98	0.45
1:E:133:HIS:O	1:E:136:ILE:HG22	2.16	0.45
1:E:475:LEU:HD13	1:E:475:LEU:O	2.17	0.45
1:H:105:THR:OG1	1:H:106:GLN:N	2.50	0.45
1:J:169:ALA:HB1	1:J:313:ALA:O	2.16	0.45
1:K:180:ARG:HD3	1:K:208:THR:OG1	2.17	0.45
1:L:54:LEU:HD13	1:L:60:ILE:HA	1.98	0.45
1:A:106:GLN:HE22	1:C:333:TYR:H	1.64	0.45
1:B:199:GLN:O	1:B:203:GLY:HA2	2.17	0.45
1:B:396:ASN:ND2	1:B:492:GLY:HA2	2.32	0.45
1:C:135:PHE:CE1	1:D:392:VAL:HG22	2.52	0.45
1:D:54:LEU:HD13	1:D:60:ILE:HA	1.99	0.45
1:D:180:ARG:HD2	1:D:206:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:LEU:HD23	1:E:51:LYS:N	2.32	0.45
1:E:239:MET:HG3	1:E:361:ILE:HG22	1.98	0.45
1:G:17:TYR:HB2	1:G:55:LYS:HE2	1.98	0.45
1:J:30:GLN:OE1	1:J:107:TYR:HB2	2.16	0.45
1:E:169:ALA:HB1	1:E:313:ALA:O	2.17	0.44
1:F:180:ARG:HA	1:F:272:THR:HG23	1.97	0.44
1:J:86:SER:O	1:J:89:TRP:N	2.40	0.44
1:A:13:VAL:HA	1:A:79:TRP:O	2.16	0.44
1:A:111:ILE:HG22	1:A:116:ILE:CD1	2.47	0.44
1:G:104:HIS:HB3	1:G:148:VAL:HG22	1.97	0.44
1:H:68:ASN:ND2	1:J:95:ILE:HD11	2.32	0.44
1:A:16:GLN:HE22	1:C:185:MET:CE	2.30	0.44
1:A:415:PRO:HD2	1:D:114:ASP:HA	2.00	0.44
1:C:380:ASP:HB3	1:C:410:ILE:HD13	2.00	0.44
1:C:490:TYR:HB2	1:D:489:LEU:HD11	1.99	0.44
1:D:10:TRP:CD2	1:D:51:LYS:HD2	2.53	0.44
1:D:54:LEU:HB3	1:D:60:ILE:HD13	1.98	0.44
1:D:458:ILE:HG12	1:D:468:TYR:CE2	2.51	0.44
1:E:150:HIS:CE1	1:E:152:GLU:HG3	2.52	0.44
1:F:150:HIS:CD2	1:F:151:TRP:CD1	3.05	0.44
1:F:363:VAL:HG23	1:F:363:VAL:O	2.17	0.44
1:F:417:LEU:HD12	1:F:418:PRO:HD2	1.99	0.44
1:G:222:PRO:HB2	1:G:225:GLU:HG3	1.98	0.44
1:H:156:VAL:O	1:H:160:ILE:HG22	2.17	0.44
1:H:162:LYS:CD	1:H:455:GLU:HG2	2.47	0.44
1:A:489:LEU:HD11	1:D:490:TYR:HB2	2.00	0.44
1:C:114:ASP:HA	1:D:415:PRO:HD2	1.99	0.44
1:C:135:PHE:HA	1:D:441:GLY:HA3	2.00	0.44
1:F:259:LEU:HB3	1:F:292:LEU:HD21	1.98	0.44
1:G:44:PHE:HE1	1:G:160:ILE:HG23	1.82	0.44
1:G:117:ASP:OD1	1:G:117:ASP:N	2.45	0.44
1:J:143:PRO:HB3	1:J:465:GLU:HG2	1.98	0.44
1:K:44:PHE:HE1	1:K:160:ILE:HG23	1.81	0.44
1:K:199:GLN:HE21	1:K:199:GLN:HB3	1.55	0.44
1:K:214:LEU:HD11	1:K:259:LEU:HD22	2.00	0.44
1:K:403:ASN:ND2	1:K:404:LYS:O	2.49	0.44
1:L:156:VAL:O	1:L:160:ILE:HG22	2.17	0.44
1:A:179:VAL:O	1:A:271:PHE:HA	2.17	0.44
1:D:7:TYR:HD2	1:D:168:CYS:HB2	1.82	0.44
1:F:47:LYS:O	1:F:48:ILE:HG13	2.17	0.44
1:G:17:TYR:N	1:G:55:LYS:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:ARG:HB2	1:G:208:THR:HA	2.00	0.44
1:I:177:GLN:OE1	1:I:207:ASN:ND2	2.49	0.44
1:J:39:ASN:HD21	1:J:48:ILE:HB	1.82	0.44
1:K:388:ASN:O	1:K:403:ASN:N	2.43	0.44
1:A:256:GLU:OE2	1:A:260:ARG:NH2	2.50	0.44
1:C:145:LYS:HD2	1:C:459:ASP:OD1	2.17	0.44
1:C:185:MET:HB3	1:C:188:VAL:HG21	1.99	0.44
1:D:314:ILE:HD12	1:D:457:LEU:HD21	1.98	0.44
1:E:326:SER:HA	1:E:351:CYS:HB3	1.99	0.44
1:G:467:GLU:HA	1:G:491:TRP:CE2	2.52	0.44
1:H:51:LYS:C	1:H:52:PRO:O	2.55	0.44
1:H:178:ILE:HA	1:H:270:GLY:O	2.16	0.44
1:B:206:ILE:CD1	1:B:305:TRP:CG	3.00	0.44
1:B:435:THR:HG23	1:B:477:LEU:HD21	2.00	0.44
1:D:92:GLY:O	1:D:95:ILE:HG22	2.18	0.44
1:E:90:ILE:HG12	1:E:136:ILE:HD11	1.99	0.44
1:E:378:VAL:HG22	1:E:418:PRO:O	2.17	0.44
1:H:80:MET:HE1	1:H:89:TRP:CH2	2.53	0.44
1:J:162:LYS:HE3	1:J:455:GLU:OE1	2.18	0.44
1:K:256:GLU:OE2	1:K:291:ARG:HB3	2.18	0.44
1:K:278:LEU:O	1:K:371:LYS:NZ	2.51	0.44
1:K:366:LEU:HD23	1:K:376:ARG:HH22	1.82	0.44
1:A:269:VAL:O	1:A:312:ARG:HD3	2.18	0.44
1:B:274:THR:HG23	1:B:277:ASP:HB3	2.00	0.44
1:C:199:GLN:HE21	1:C:199:GLN:HB3	1.69	0.44
1:C:403:ASN:HD21	1:C:426:PRO:HB3	1.83	0.44
1:E:418:PRO:HG3	1:F:118:MET:HG2	2.00	0.44
1:F:50:LEU:HD23	1:F:51:LYS:N	2.32	0.44
1:F:56:SER:HB3	1:F:59:GLU:HG3	2.00	0.44
1:H:184:ASN:HA	1:H:303:GLY:HA3	2.00	0.44
1:J:35:VAL:HG21	1:J:50:LEU:HB2	2.00	0.44
1:J:133:HIS:O	1:J:136:ILE:HG22	2.18	0.44
1:K:12:LEU:HD12	1:K:12:LEU:HA	1.86	0.44
1:K:410:ILE:HG13	1:K:423:LEU:HD12	1.99	0.44
1:L:326:SER:OG	1:L:327:PHE:N	2.50	0.44
1:B:38:LEU:HB3	1:B:48:ILE:HD12	2.00	0.44
1:C:376:ARG:HD2	1:C:418:PRO:HB2	2.00	0.44
1:D:159:LYS:HG3	1:D:455:GLU:OE2	2.17	0.44
1:E:290:GLN:HE21	1:E:350:VAL:H	1.65	0.44
1:E:460:TRP:O	1:E:463:ALA:N	2.51	0.44
1:F:162:LYS:HD2	1:F:455:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:LEU:HD11	1:F:259:LEU:HD22	1.99	0.44
1:F:274:THR:HG23	1:F:277:ASP:HB3	2.00	0.44
1:G:4:LEU:HD11	1:G:45:PRO:HB2	2.00	0.44
1:H:34:ILE:HD11	1:H:107:TYR:HB2	2.00	0.44
1:H:169:ALA:HB1	1:H:313:ALA:O	2.18	0.44
1:I:482:LYS:HB3	1:I:486:TRP:CZ3	2.53	0.44
1:L:248:ALA:HB1	1:L:283:GLN:HE22	1.83	0.44
1:A:114:ASP:OD1	1:A:114:ASP:N	2.51	0.43
1:B:429:ASP:HB3	1:B:432:ARG:HD2	2.00	0.43
1:C:408:VAL:HG11	1:C:425:LYS:HE3	2.00	0.43
1:D:380:ASP:CG	1:D:410:ILE:HD13	2.39	0.43
1:E:155:GLU:O	1:E:158:GLU:HB2	2.17	0.43
1:F:206:ILE:CD1	1:F:305:TRP:CG	3.01	0.43
1:H:78:VAL:HG11	1:H:133:HIS:NE2	2.33	0.43
1:H:373:ASP:OD1	1:H:373:ASP:N	2.50	0.43
1:I:68:ASN:ND2	1:I:98:LYS:HD3	2.33	0.43
1:J:143:PRO:HB3	1:J:465:GLU:OE2	2.18	0.43
1:J:151:TRP:O	1:J:157:ARG:NE	2.51	0.43
1:A:189:ALA:HB2	1:D:87:LYS:HG3	2.00	0.43
1:A:211:VAL:HG11	1:A:278:LEU:HA	2.00	0.43
1:B:287:LEU:HA	1:B:290:GLN:OE1	2.18	0.43
1:D:77:ILE:HD13	1:D:160:ILE:HD11	1.99	0.43
1:G:130:ASP:HA	1:G:133:HIS:HB3	2.00	0.43
1:L:315:LYS:NZ	1:L:351:CYS:SG	2.88	0.43
1:A:249:ILE:HD13	1:A:361:ILE:HG21	2.00	0.43
1:B:111:ILE:HG22	1:B:116:ILE:HG21	2.00	0.43
1:C:80:MET:CG	1:C:130:ASP:HB3	2.49	0.43
1:D:237:TYR:HB2	1:D:238:ILE:H	1.65	0.43
1:E:431:LYS:HE2	1:F:153:GLU:OE2	2.18	0.43
1:G:50:LEU:C	1:G:50:LEU:CD2	2.86	0.43
1:I:180:ARG:HA	1:I:272:THR:HG23	2.00	0.43
1:K:37:SER:O	1:K:157:ARG:NH2	2.52	0.43
1:K:320:SER:OG	1:K:322:PRO:HD2	2.17	0.43
1:K:363:VAL:HG23	1:K:363:VAL:O	2.18	0.43
1:A:141:ARG:NH2	1:C:394:MET:O	2.51	0.43
1:A:395:GLY:HA2	1:D:139:ARG:HH11	1.83	0.43
1:B:269:VAL:HB	1:B:312:ARG:NE	2.33	0.43
1:C:279:HIS:CD2	1:G:213:GLU:HG2	2.54	0.43
1:C:314:ILE:HG23	1:C:325:THR:HG21	2.00	0.43
1:D:133:HIS:O	1:D:136:ILE:HG22	2.17	0.43
1:E:174:ARG:HG2	1:E:203:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:LEU:HD22	1:E:391:ILE:HG13	2.00	0.43
1:F:342:VAL:HG11	1:F:424:TRP:NE1	2.34	0.43
1:G:156:VAL:O	1:G:160:ILE:HG22	2.18	0.43
1:I:50:LEU:HD23	1:I:51:LYS:O	2.17	0.43
1:I:211:VAL:HG21	1:I:277:ASP:O	2.17	0.43
1:A:239:MET:CB	1:A:240:PRO:HD3	2.45	0.43
1:A:377:LEU:O	1:A:420:ALA:HB2	2.17	0.43
1:A:399:ARG:NH1	1:A:440:ALA:O	2.49	0.43
1:B:2:ILE:O	1:B:2:ILE:HG22	2.18	0.43
1:B:243:GLU:C	1:B:245:SER:H	2.22	0.43
1:B:402:VAL:HG13	1:B:470:VAL:HA	2.00	0.43
1:C:54:LEU:HD21	1:C:63:ILE:HG13	2.00	0.43
1:C:86:SER:OG	1:C:133:HIS:HA	2.18	0.43
1:C:111:ILE:O	1:C:113:TRP:N	2.52	0.43
1:C:147:VAL:CG1	1:C:156:VAL:HG23	2.48	0.43
1:C:247:LYS:O	1:C:247:LYS:HG2	2.18	0.43
1:D:140:MET:HB3	1:D:142:LEU:HD23	2.00	0.43
1:G:80:MET:HE1	1:G:89:TRP:CZ2	2.54	0.43
1:J:54:LEU:HB3	1:J:60:ILE:HD13	2.01	0.43
1:L:256:GLU:OE2	1:L:291:ARG:NH2	2.50	0.43
1:L:325:THR:HA	1:L:449:SER:HA	2.00	0.43
1:A:30:GLN:HE22	1:A:123:LEU:HD21	1.83	0.43
1:A:111:ILE:HD11	1:C:334:HIS:HB2	2.01	0.43
1:B:29:GLN:HG3	1:F:110:GLU:HB2	2.01	0.43
1:C:87:LYS:HA	1:C:90:ILE:HD12	2.01	0.43
1:A:61:THR:HA	1:A:92:GLY:HA2	2.01	0.43
1:A:180:ARG:HA	1:A:272:THR:HG22	2.01	0.43
1:E:201:LYS:NZ	1:E:495:LYS:HG2	2.34	0.43
1:F:431:LYS:HE2	1:G:153:GLU:OE2	2.19	0.43
1:G:343:LEU:HD11	1:G:421:ARG:HB2	2.01	0.43
1:I:334:HIS:HB3	1:I:341:LEU:HB2	2.00	0.43
1:J:56:SER:O	1:J:60:ILE:HG12	2.17	0.43
1:L:274:THR:HG23	1:L:277:ASP:HB3	2.01	0.43
1:C:381:GLY:HA3	1:C:422:VAL:HA	2.01	0.43
1:D:15:SER:HA	1:D:82:THR:HG23	2.00	0.43
1:F:310:LEU:HB2	1:F:391:ILE:HD12	2.01	0.43
1:F:438:ILE:HG23	1:G:134:GLY:HA3	2.00	0.43
1:J:195:LYS:HG3	1:J:206:ILE:HD13	2.01	0.43
1:B:417:LEU:HD23	1:B:421:ARG:HE	1.84	0.43
1:C:246:LEU:HA	1:C:249:ILE:HG12	2.00	0.43
1:D:239:MET:SD	1:D:245:SER:HB3	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:SER:O	1:F:323:GLY:N	2.52	0.43
1:F:342:VAL:HG12	1:F:424:TRP:O	2.18	0.43
1:G:154:LYS:HE2	1:G:158:GLU:OE1	2.19	0.43
1:H:20:GLY:O	1:H:23:THR:HG22	2.19	0.43
1:J:271:PHE:O	1:J:299:PHE:HA	2.18	0.43
1:A:104:HIS:CD2	1:C:438:ILE:HD11	2.54	0.43
1:A:166:VAL:HG13	1:A:460:TRP:HD1	1.84	0.43
1:A:299:PHE:CG	1:A:300:GLY:N	2.86	0.43
1:B:109:ARG:HG3	1:B:150:HIS:ND1	2.34	0.43
1:B:405:VAL:HB	1:B:424:TRP:CD1	2.54	0.43
1:D:30:GLN:OE1	1:D:107:TYR:HB2	2.19	0.43
1:D:339:ASN:OD1	1:D:425:LYS:HE2	2.18	0.43
1:E:162:LYS:O	1:E:166:VAL:HG23	2.19	0.43
1:E:426:PRO:HB2	1:E:433:ALA:HB3	2.00	0.43
1:H:201:LYS:HE3	1:H:465:GLU:O	2.18	0.43
1:I:305:TRP:HA	1:I:308:ALA:HB3	2.01	0.43
1:J:16:GLN:C	1:J:55:LYS:HB2	2.39	0.43
1:K:177:GLN:OE1	1:K:207:ASN:ND2	2.48	0.43
1:B:321:LEU:O	1:B:323:GLY:N	2.52	0.42
1:F:183:ASP:OD1	1:F:184:ASN:N	2.38	0.42
1:I:140:MET:HB3	1:I:142:LEU:HD23	2.00	0.42
1:J:417:LEU:HD12	1:J:418:PRO:HD2	2.01	0.42
1:B:56:SER:HB3	1:B:59:GLU:HG3	2.00	0.42
1:C:141:ARG:NH2	1:D:394:MET:O	2.52	0.42
1:D:396:ASN:HB3	1:E:396:ASN:HB3	2.01	0.42
1:F:382:GLN:O	1:F:407:SER:OG	2.23	0.42
1:H:214:LEU:HD11	1:H:259:LEU:HD22	2.00	0.42
1:I:399:ARG:NH1	1:I:484:LEU:HD22	2.33	0.42
1:J:8:GLU:OE1	1:J:49:VAL:HG21	2.20	0.42
1:J:101:LEU:HD13	1:J:160:ILE:HG13	2.01	0.42
1:K:184:ASN:HA	1:K:303:GLY:HA3	2.01	0.42
1:L:130:ASP:HA	1:L:133:HIS:HB3	2.01	0.42
1:L:214:LEU:HD11	1:L:259:LEU:HD22	2.02	0.42
1:L:314:ILE:HD11	1:L:452:ILE:HD11	2.00	0.42
1:L:326:SER:HA	1:L:351:CYS:HB3	2.00	0.42
1:A:86:SER:O	1:A:89:TRP:N	2.52	0.42
1:C:179:VAL:O	1:C:271:PHE:HA	2.19	0.42
1:D:60:ILE:HD12	1:D:89:TRP:CD2	2.54	0.42
1:K:104:HIS:HA	1:K:130:ASP:OD2	2.19	0.42
1:K:195:LYS:HG3	1:K:206:ILE:HD13	2.00	0.42
1:A:252:GLN:HG2	1:A:283:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:HD12	1:B:12:LEU:HA	1.81	0.42
1:C:172:ASP:OD2	1:C:316:VAL:HG21	2.19	0.42
1:C:490:TYR:CE1	1:D:485:ARG:HB2	2.53	0.42
1:D:432:ARG:O	1:D:435:THR:HG22	2.19	0.42
1:F:356:LYS:HD3	1:F:382:GLN:HA	2.02	0.42
1:G:314:ILE:HG23	1:G:325:THR:HG21	2.01	0.42
1:J:232:GLU:O	1:J:235:GLU:HB2	2.19	0.42
1:J:388:ASN:ND2	1:J:424:TRP:CZ2	2.87	0.42
1:K:7:TYR:O	1:K:46:SER:HB3	2.19	0.42
1:K:166:VAL:HG21	1:K:456:TYR:O	2.18	0.42
1:L:1:MET:HA	1:L:295:GLU:O	2.20	0.42
1:L:273:THR:HG22	1:L:299:PHE:CE1	2.54	0.42
1:B:12:LEU:HD11	1:B:63:ILE:HG21	2.02	0.42
1:D:199:GLN:CD	1:D:205:SER:HA	2.40	0.42
1:E:87:LYS:HB2	1:G:187:GLU:O	2.20	0.42
1:E:184:ASN:ND2	1:E:192:GLU:CD	2.73	0.42
1:F:107:TYR:CE2	1:F:124:ASN:ND2	2.86	0.42
1:F:206:ILE:HD12	1:F:305:TRP:CG	2.55	0.42
1:G:477:LEU:HD22	1:G:477:LEU:HA	1.92	0.42
1:J:493:LEU:HD23	1:J:493:LEU:H	1.83	0.42
1:K:202:LEU:HD22	1:K:464:LEU:HD13	2.01	0.42
1:L:8:GLU:OE1	1:L:49:VAL:HG21	2.20	0.42
1:A:102:HIS:NE2	1:A:130:ASP:HB2	2.34	0.42
1:B:57:SER:HA	1:B:88:MET:HB3	2.01	0.42
1:B:177:GLN:HG2	1:B:178:ILE:O	2.20	0.42
1:B:284:LEU:HD12	1:B:285:PRO:HD2	2.02	0.42
1:B:493:LEU:HD23	1:B:493:LEU:H	1.85	0.42
1:D:124:ASN:C	1:D:126:SER:H	2.22	0.42
1:D:321:LEU:O	1:D:323:GLY:N	2.53	0.42
1:E:461:ALA:HA	1:E:466:ILE:HG12	2.02	0.42
1:F:201:LYS:HE3	1:F:464:LEU:O	2.20	0.42
1:F:259:LEU:O	1:F:262:PHE:N	2.51	0.42
1:F:389:ALA:HA	1:F:402:VAL:HA	2.02	0.42
1:G:139:ARG:O	1:G:139:ARG:HD3	2.19	0.42
1:I:180:ARG:HB2	1:I:208:THR:HG23	2.02	0.42
1:I:216:GLU:O	1:I:219:LYS:HG3	2.19	0.42
1:K:321:LEU:C	1:K:323:GLY:H	2.22	0.42
1:C:28:GLU:HG2	1:C:53:VAL:CG2	2.49	0.42
1:C:38:LEU:HD12	1:C:38:LEU:HA	1.96	0.42
1:C:304:ASP:HB2	1:C:445:HIS:HD1	1.85	0.42
1:E:101:LEU:HD13	1:E:160:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:GLN:O	1:E:150:HIS:CD2	2.72	0.42
1:F:20:GLY:O	1:F:23:THR:HG22	2.19	0.42
1:G:86:SER:O	1:G:89:TRP:N	2.42	0.42
1:G:169:ALA:HA	1:G:316:VAL:HG11	2.02	0.42
1:J:107:TYR:O	1:J:150:HIS:NE2	2.46	0.42
1:J:122:ASN:OD1	1:K:368:ILE:HD11	2.19	0.42
1:L:56:SER:O	1:L:60:ILE:HG12	2.19	0.42
1:L:315:LYS:O	1:L:318:GLY:N	2.52	0.42
1:A:462:GLU:OE1	1:C:481:LYS:HE3	2.20	0.42
1:B:102:HIS:NE2	1:B:130:ASP:HB2	2.35	0.42
1:B:157:ARG:HA	1:B:160:ILE:CG2	2.49	0.42
1:C:273:THR:HG22	1:C:299:PHE:CE1	2.54	0.42
1:E:404:LYS:HD3	1:E:473:GLU:OE2	2.19	0.42
1:E:416:LYS:HG3	1:F:117:ASP:HB3	2.02	0.42
1:F:180:ARG:HB2	1:F:208:THR:HG23	2.00	0.42
1:F:321:LEU:C	1:F:323:GLY:N	2.72	0.42
1:F:435:THR:HG23	1:F:477:LEU:HD21	2.01	0.42
1:H:236:LYS:HB3	1:H:237:TYR:CE1	2.55	0.42
1:H:314:ILE:HG23	1:H:325:THR:HG21	2.00	0.42
1:J:270:GLY:HA2	1:J:298:GLY:O	2.19	0.42
1:A:28:GLU:HG2	1:A:53:VAL:HG23	2.01	0.42
1:A:180:ARG:HD3	1:A:208:THR:OG1	2.20	0.42
1:D:306:LYS:H	1:D:306:LYS:HG2	1.61	0.42
1:F:163:TRP:O	1:F:164:MET:C	2.58	0.42
1:F:209:TRP:CZ2	1:F:266:LYS:HG2	2.54	0.42
1:F:366:LEU:HD12	1:F:366:LEU:O	2.20	0.42
1:G:54:LEU:HD13	1:G:60:ILE:HD13	2.01	0.42
1:H:439:LEU:HD23	1:H:439:LEU:HA	1.90	0.42
1:J:15:SER:OG	1:J:16:GLN:N	2.43	0.42
1:L:233:TYR:HB3	1:L:238:ILE:HG12	2.02	0.42
1:B:61:THR:HA	1:B:92:GLY:HA2	2.02	0.42
1:C:92:GLY:O	1:C:95:ILE:HG22	2.19	0.42
1:F:10:TRP:CE3	1:F:51:LYS:HD2	2.55	0.42
1:G:77:ILE:HD13	1:G:160:ILE:HD11	2.02	0.42
1:I:405:VAL:HG12	1:I:426:PRO:HA	2.01	0.42
1:J:108:ASN:ND2	1:J:120:TYR:OH	2.50	0.42
1:K:180:ARG:HD2	1:K:206:ILE:HD11	2.02	0.42
1:K:314:ILE:HG23	1:K:325:THR:HG21	2.01	0.42
1:C:194:ASP:HB3	1:C:197:GLU:HB3	2.01	0.41
1:D:239:MET:O	1:D:240:PRO:C	2.58	0.41
1:F:478:GLU:OE2	1:G:468:TYR:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:TRP:CH2	1:G:266:LYS:HG2	2.55	0.41
1:H:270:GLY:HA2	1:H:298:GLY:O	2.20	0.41
1:I:278:LEU:HD13	1:I:284:LEU:HA	2.02	0.41
1:J:87:LYS:HA	1:J:90:ILE:CD1	2.50	0.41
1:K:165:ARG:HA	1:K:168:CYS:SG	2.59	0.41
1:L:328:MET:HB2	1:L:448:PHE:HB2	2.01	0.41
1:B:410:ILE:HG22	1:B:412:ARG:O	2.20	0.41
1:C:215:ALA:O	1:C:218:VAL:HG22	2.20	0.41
1:C:327:PHE:HE1	1:C:445:HIS:HB3	1.85	0.41
1:F:32:SER:O	1:F:36:ASP:HB2	2.19	0.41
1:I:279:HIS:CD2	1:J:213:GLU:HG2	2.55	0.41
1:I:482:LYS:O	1:I:485:ARG:HG2	2.20	0.41
1:J:378:VAL:HG22	1:J:418:PRO:O	2.20	0.41
1:A:186:ARG:HD3	1:F:208:THR:O	2.20	0.41
1:A:299:PHE:O	1:A:308:ALA:HA	2.20	0.41
1:C:410:ILE:HA	1:C:423:LEU:HD12	2.01	0.41
1:C:467:GLU:HA	1:C:491:TRP:CE2	2.54	0.41
1:D:82:THR:OG1	1:D:83:PHE:N	2.51	0.41
1:D:192:GLU:OE1	1:E:195:LYS:HD3	2.19	0.41
1:D:246:LEU:HA	1:D:249:ILE:HG12	2.02	0.41
1:E:333:TYR:HB2	1:F:106:GLN:OE1	2.20	0.41
1:F:79:TRP:HB2	1:F:103:LEU:HB3	2.02	0.41
1:H:298:GLY:HA3	1:H:312:ARG:HB2	2.02	0.41
1:I:107:TYR:HA	1:I:151:TRP:HE1	1.85	0.41
1:L:273:THR:HG22	1:L:299:PHE:CZ	2.55	0.41
1:A:389:ALA:HB1	1:A:400:LEU:HD11	2.01	0.41
1:B:239:MET:O	1:B:240:PRO:C	2.59	0.41
1:D:363:VAL:HG23	1:D:363:VAL:O	2.20	0.41
1:E:330:ASP:OD1	1:E:330:ASP:N	2.53	0.41
1:F:34:ILE:HG12	1:F:151:TRP:CE2	2.56	0.41
1:F:209:TRP:CZ2	1:F:266:LYS:HE2	2.56	0.41
1:G:195:LYS:HG3	1:G:206:ILE:HD13	2.02	0.41
1:H:54:LEU:HD22	1:H:59:GLU:HB3	2.03	0.41
1:I:161:ALA:O	1:I:164:MET:HB2	2.20	0.41
1:K:39:ASN:OD1	1:K:48:ILE:HB	2.20	0.41
1:K:162:LYS:HD2	1:K:455:GLU:HG2	2.02	0.41
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.93	0.41
1:C:180:ARG:HA	1:C:272:THR:HG23	2.01	0.41
1:D:256:GLU:OE2	1:D:291:ARG:HB3	2.21	0.41
1:E:214:LEU:HD11	1:E:259:LEU:HD22	2.03	0.41
1:G:21:LEU:HD12	1:G:24:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:467:GLU:HB2	1:G:491:TRP:CD1	2.56	0.41
1:H:262:PHE:HD1	1:H:266:LYS:HG3	1.86	0.41
1:I:259:LEU:O	1:I:263:LEU:HG	2.20	0.41
1:J:78:VAL:HG23	1:J:100:LEU:HD12	2.02	0.41
1:K:160:ILE:HG12	1:K:164:MET:HE3	2.03	0.41
1:C:17:TYR:N	1:C:55:LYS:HB2	2.35	0.41
1:C:199:GLN:CD	1:C:205:SER:HA	2.41	0.41
1:C:302:GLU:HB2	1:C:445:HIS:HE1	1.86	0.41
1:D:472:ASP:O	1:D:475:LEU:HB2	2.21	0.41
1:E:228:GLU:O	1:E:231:LYS:HG2	2.21	0.41
1:F:158:GLU:O	1:F:159:LYS:C	2.58	0.41
1:H:389:ALA:HA	1:H:402:VAL:HA	2.03	0.41
1:B:96:ASN:ND2	1:B:100:LEU:HD21	2.36	0.41
1:C:227:GLU:HA	1:C:230:LEU:HB2	2.03	0.41
1:E:408:VAL:HG11	1:E:425:LYS:HE3	2.02	0.41
1:F:326:SER:CB	1:F:351:CYS:HB3	2.51	0.41
1:J:273:THR:OG1	1:J:274:THR:N	2.53	0.41
1:J:326:SER:OG	1:J:327:PHE:N	2.54	0.41
1:K:38:LEU:HD12	1:K:157:ARG:HH21	1.86	0.41
1:K:227:GLU:HA	1:K:230:LEU:HB2	2.03	0.41
1:L:50:LEU:HD23	1:L:51:LYS:N	2.35	0.41
1:C:248:ALA:HB3	1:C:363:VAL:HG11	2.03	0.41
1:C:493:LEU:HD23	1:C:493:LEU:H	1.86	0.41
1:D:145:LYS:HE2	1:D:163:TRP:HB2	2.02	0.41
1:E:104:HIS:CE1	1:E:130:ASP:OD1	2.74	0.41
1:G:86:SER:HA	1:G:89:TRP:HD1	1.85	0.41
1:H:153:GLU:HG2	1:H:154:LYS:N	2.35	0.41
1:J:56:SER:HB3	1:J:59:GLU:HG3	2.03	0.41
1:K:405:VAL:HG12	1:K:426:PRO:HA	2.02	0.41
1:K:429:ASP:OD1	1:K:430:PHE:N	2.53	0.41
1:B:51:LYS:HD3	1:B:63:ILE:HG23	2.03	0.41
1:C:100:LEU:HB3	1:C:144:ARG:HB2	2.03	0.41
1:D:390:SER:HB3	1:D:437:TRP:CH2	2.55	0.41
1:E:450:THR:O	1:E:450:THR:HG22	2.21	0.41
1:E:467:GLU:OE2	1:E:487:ASN:CB	2.69	0.41
1:F:241:GLU:HG2	1:F:242:ASP:H	1.86	0.41
1:G:215:ALA:O	1:G:218:VAL:HG22	2.21	0.41
1:H:124:ASN:C	1:H:126:SER:H	2.24	0.41
1:H:150:HIS:HB2	1:I:335:LEU:HB3	2.03	0.41
1:H:293:MET:O	1:H:315:LYS:NZ	2.37	0.41
1:I:12:LEU:HA	1:I:12:LEU:HD12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4:LEU:O	1:J:46:SER:OG	2.39	0.41
1:J:104:HIS:HD1	1:J:130:ASP:CG	2.24	0.41
1:J:162:LYS:HG2	1:J:456:TYR:CZ	2.56	0.41
1:J:249:ILE:HD12	1:J:361:ILE:HD13	2.03	0.41
1:J:305:TRP:HA	1:J:308:ALA:HB3	2.03	0.41
1:J:364:HIS:HA	1:J:365:PRO:HD3	1.96	0.41
1:J:402:VAL:HG13	1:J:470:VAL:HA	2.02	0.41
1:K:184:ASN:HD22	1:K:192:GLU:CD	2.24	0.41
1:K:236:LYS:HB3	1:K:237:TYR:CE1	2.55	0.41
1:L:12:LEU:HD11	1:L:54:LEU:HD11	2.02	0.41
1:L:324:GLY:HA2	1:L:353:THR:HG22	2.02	0.41
1:A:224:ARG:HG2	1:A:227:GLU:OE2	2.21	0.41
1:C:15:SER:O	1:C:55:LYS:HA	2.21	0.41
1:D:8:GLU:HG2	1:D:72:LYS:O	2.20	0.41
1:F:400:LEU:O	1:F:400:LEU:HG	2.21	0.41
1:H:201:LYS:NZ	1:H:495:LYS:HG2	2.35	0.41
1:I:80:MET:SD	1:I:84:SER:OG	2.62	0.41
1:J:14:GLY:HA3	1:J:89:TRP:HZ2	1.86	0.41
1:J:278:LEU:O	1:J:281:LEU:HB2	2.21	0.41
1:K:80:MET:HG2	1:K:130:ASP:HB3	2.03	0.41
1:K:315:LYS:HD3	1:K:325:THR:HB	2.03	0.41
1:L:340:GLU:O	1:L:340:GLU:CG	2.69	0.41
1:A:180:ARG:HB2	1:A:208:THR:HG23	2.02	0.40
1:C:283:GLN:NE2	1:C:373:ASP:O	2.54	0.40
1:C:328:MET:HB2	1:C:448:PHE:HB2	2.02	0.40
1:E:281:LEU:HD23	1:E:281:LEU:HA	1.98	0.40
1:H:38:LEU:HG	1:H:44:PHE:CE2	2.55	0.40
1:H:143:PRO:HB3	1:H:465:GLU:HG2	2.02	0.40
1:I:439:LEU:HD23	1:I:439:LEU:HA	1.95	0.40
1:J:79:TRP:CZ2	1:J:81:HIS:HA	2.56	0.40
1:K:133:HIS:O	1:K:136:ILE:HG22	2.20	0.40
1:L:73:CYS:O	1:L:73:CYS:SG	2.80	0.40
1:A:127:ALA:HB2	1:C:333:TYR:CZ	2.56	0.40
1:A:177:GLN:HG2	1:A:178:ILE:O	2.21	0.40
1:B:6:GLN:HG3	1:B:7:TYR:N	2.34	0.40
1:C:34:ILE:O	1:C:38:LEU:HB2	2.22	0.40
1:C:346:HIS:ND1	1:C:347:MET:HG2	2.36	0.40
1:D:284:LEU:HD12	1:D:285:PRO:HD2	2.03	0.40
1:F:61:THR:HA	1:F:92:GLY:HA2	2.02	0.40
1:F:314:ILE:HG23	1:F:325:THR:HG21	2.03	0.40
1:H:50:LEU:HD23	1:H:51:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:484:LEU:HD23	1:H:484:LEU:HA	1.93	0.40
1:I:16:GLN:C	1:I:55:LYS:HB2	2.42	0.40
1:I:136:ILE:HD12	1:I:136:ILE:HA	1.96	0.40
1:I:156:VAL:O	1:I:160:ILE:HG22	2.20	0.40
1:K:237:TYR:HB2	1:K:238:ILE:H	1.67	0.40
1:D:311:VAL:HA	1:D:314:ILE:HG22	2.02	0.40
1:F:310:LEU:HD13	1:F:391:ILE:HD11	2.04	0.40
1:F:405:VAL:HG12	1:F:426:PRO:HA	2.01	0.40
1:G:432:ARG:O	1:G:435:THR:HG22	2.20	0.40
1:G:482:LYS:HB3	1:G:486:TRP:CZ3	2.57	0.40
1:H:140:MET:HB3	1:H:142:LEU:HD23	2.03	0.40
1:I:57:SER:O	1:I:61:THR:HG23	2.21	0.40
1:I:228:GLU:HG3	1:I:231:LYS:HD3	2.03	0.40
1:I:284:LEU:HD12	1:I:285:PRO:HD2	2.02	0.40
1:L:278:LEU:HD11	1:L:284:LEU:HD12	2.03	0.40
1:A:391:ILE:HD11	1:A:460:TRP:CH2	2.57	0.40
1:B:156:VAL:O	1:B:160:ILE:HG22	2.20	0.40
1:B:279:HIS:NE2	1:L:213:GLU:HG2	2.36	0.40
1:D:304:ASP:OD1	1:D:307:ALA:HB3	2.20	0.40
1:E:86:SER:CB	1:E:132:GLU:OE2	2.69	0.40
1:E:96:ASN:OD1	1:E:98:LYS:N	2.48	0.40
1:E:328:MET:HB2	1:E:448:PHE:HB2	2.03	0.40
1:E:473:GLU:H	1:E:473:GLU:CD	2.25	0.40
1:F:130:ASP:OD1	1:F:130:ASP:N	2.54	0.40
1:G:10:TRP:CE3	1:G:67:ALA:HB2	2.57	0.40
1:G:223:GLU:O	1:G:226:VAL:HG22	2.22	0.40
1:G:239:MET:O	1:G:240:PRO:C	2.60	0.40
1:H:30:GLN:OE1	1:H:81:HIS:NE2	2.46	0.40
1:H:118:MET:HG2	1:I:418:PRO:HG3	2.03	0.40
1:H:223:GLU:O	1:H:226:VAL:HG22	2.22	0.40
1:H:380:ASP:HB3	1:H:410:ILE:HD13	2.03	0.40
1:H:386:ALA:HB1	1:H:449:SER:O	2.21	0.40
1:I:252:GLN:HG3	1:I:375:ALA:HB3	2.03	0.40
1:I:476:ASP:HB3	1:I:479:ASP:HB2	2.02	0.40
1:J:38:LEU:HG	1:J:44:PHE:CE2	2.56	0.40
1:J:274:THR:HG23	1:J:277:ASP:HB3	2.02	0.40
1:L:399:ARG:NH1	1:L:484:LEU:HD22	2.37	0.40
1:A:192:GLU:O	1:A:306:LYS:NZ	2.52	0.40
1:B:12:LEU:HD11	1:B:54:LEU:HD11	2.04	0.40
1:B:22:GLU:HG3	1:E:412:ARG:HD3	2.02	0.40
1:B:351:CYS:HA	1:B:352:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LYS:HD3	1:C:63:ILE:HD12	2.03	0.40
1:C:396:ASN:OD1	1:C:396:ASN:N	2.54	0.40
1:F:3:ASP:OD1	1:F:3:ASP:C	2.59	0.40
1:F:311:VAL:O	1:F:315:LYS:HB2	2.22	0.40
1:H:106:GLN:HB3	1:I:335:LEU:HD21	2.04	0.40
1:I:272:THR:OG1	1:I:300:GLY:O	2.29	0.40
1:J:321:LEU:C	1:J:323:GLY:H	2.24	0.40
1:K:296:GLY:O	1:K:297:TYR:C	2.60	0.40
1:K:477:LEU:HD22	1:K:477:LEU:HA	1.93	0.40
1:L:60:ILE:HD12	1:L:89:TRP:CD2	2.57	0.40
1:L:480:PHE:O	1:L:483:GLU:HB3	2.21	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	487/496 (98%)	412 (85%)	67 (14%)	8 (2%)	9	46
1	B	492/496 (99%)	433 (88%)	48 (10%)	11 (2%)	6	39
1	C	483/496 (97%)	426 (88%)	46 (10%)	11 (2%)	6	38
1	D	493/496 (99%)	434 (88%)	44 (9%)	15 (3%)	4	33
1	E	493/496 (99%)	430 (87%)	49 (10%)	14 (3%)	5	34
1	F	493/496 (99%)	428 (87%)	53 (11%)	12 (2%)	6	37
1	G	493/496 (99%)	427 (87%)	56 (11%)	10 (2%)	7	42
1	H	493/496 (99%)	428 (87%)	55 (11%)	10 (2%)	7	42
1	I	493/496 (99%)	426 (86%)	54 (11%)	13 (3%)	5	35
1	J	493/496 (99%)	426 (86%)	56 (11%)	11 (2%)	6	39
1	K	493/496 (99%)	432 (88%)	50 (10%)	11 (2%)	6	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	493/496 (99%)	439 (89%)	45 (9%)	9 (2%)	8	43
All	All	5899/5952 (99%)	5141 (87%)	623 (11%)	135 (2%)	6	38

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	GLY
1	B	323	GLY
1	C	238	ILE
1	D	242	ASP
1	D	323	GLY
1	D	428	PRO
1	E	323	GLY
1	E	395	GLY
1	E	428	PRO
1	F	240	PRO
1	G	323	GLY
1	I	267	ASN
1	I	323	GLY
1	I	428	PRO
1	L	267	ASN
1	A	238	ILE
1	B	238	ILE
1	B	240	PRO
1	C	18	LEU
1	C	304	ASP
1	D	183	ASP
1	D	238	ILE
1	D	240	PRO
1	D	370	GLY
1	E	173	GLY
1	E	238	ILE
1	F	238	ILE
1	F	297	TYR
1	F	323	GLY
1	G	238	ILE
1	G	370	GLY
1	H	238	ILE
1	H	323	GLY
1	H	340	GLU
1	H	395	GLY
1	I	238	ILE

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Mol	Chain	Res	Type
1	I	286	GLY
1	I	395	GLY
1	I	465	GLU
1	J	238	ILE
1	J	323	GLY
1	J	348	LEU
1	J	492	GLY
1	K	238	ILE
1	K	297	TYR
1	L	238	ILE
1	L	242	ASP
1	L	348	LEU
1	L	428	PRO
1	A	330	ASP
1	A	372	ALA
1	A	492	GLY
1	B	304	ASP
1	C	173	GLY
1	C	286	GLY
1	C	345	ALA
1	C	348	LEU
1	E	18	LEU
1	E	348	LEU
1	E	460	TRP
1	F	286	GLY
1	F	348	LEU
1	F	413	LYS
1	G	340	GLU
1	I	22	GLU
1	I	240	PRO
1	I	348	LEU
1	K	240	PRO
1	K	242	ASP
1	K	324	GLY
1	K	348	LEU
1	L	240	PRO
1	A	348	LEU
1	B	127	ALA
1	B	322	PRO
1	B	370	GLY
1	B	428	PRO
1	C	322	PRO

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Mol	Chain	Res	Type
1	C	428	PRO
1	D	286	GLY
1	D	348	LEU
1	E	183	ASP
1	E	324	GLY
1	E	370	GLY
1	F	18	LEU
1	F	242	ASP
1	G	240	PRO
1	G	348	LEU
1	G	428	PRO
1	H	52	PRO
1	H	304	ASP
1	H	348	LEU
1	J	428	PRO
1	K	428	PRO
1	K	492	GLY
1	B	183	ASP
1	B	204	TRP
1	B	348	LEU
1	C	112	PRO
1	C	127	ALA
1	D	330	ASP
1	D	345	ALA
1	E	151	TRP
1	E	240	PRO
1	G	15	SER
1	H	324	GLY
1	I	345	ALA
1	J	18	LEU
1	J	240	PRO
1	J	456	TYR
1	K	322	PRO
1	K	330	ASP
1	L	323	GLY
1	D	304	ASP
1	D	322	PRO
1	E	286	GLY
1	G	286	GLY
1	J	34	ILE
1	J	183	ASP
1	K	340	GLU

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Mol	Chain	Res	Type
1	L	18	LEU
1	D	296	GLY
1	F	322	PRO
1	I	173	GLY
1	L	116	ILE
1	F	112	PRO
1	G	322	PRO
1	A	239	MET
1	D	368	ILE
1	J	173	GLY
1	H	92	GLY
1	I	296	GLY
1	F	428	PRO
1	A	428	PRO
1	H	428	PRO

5.3.2 Protein sidechains [i](#)

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	421/426 (99%)	397 (94%)	24 (6%)	20	55
1	B	424/426 (100%)	407 (96%)	17 (4%)	31	65
1	C	420/426 (99%)	399 (95%)	21 (5%)	24	59
1	D	425/426 (100%)	406 (96%)	19 (4%)	27	62
1	E	425/426 (100%)	405 (95%)	20 (5%)	26	61
1	F	425/426 (100%)	397 (93%)	28 (7%)	16	50
1	G	425/426 (100%)	397 (93%)	28 (7%)	16	50
1	H	425/426 (100%)	401 (94%)	24 (6%)	21	55
1	I	425/426 (100%)	409 (96%)	16 (4%)	33	66
1	J	425/426 (100%)	400 (94%)	25 (6%)	19	54
1	K	425/426 (100%)	401 (94%)	24 (6%)	21	55
1	L	425/426 (100%)	405 (95%)	20 (5%)	26	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5090/5112 (100%)	4824 (95%)	266 (5%)	23 58

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	40	ASP
1	A	91	ARG
1	A	98	LYS
1	A	107	TYR
1	A	114	ASP
1	A	120	TYR
1	A	139	ARG
1	A	144	ARG
1	A	219	LYS
1	A	223	GLU
1	A	234	ARG
1	A	236	LYS
1	A	237	TYR
1	A	245	SER
1	A	247	LYS
1	A	330	ASP
1	A	331	TYR
1	A	394	MET
1	A	419	THR
1	A	421	ARG
1	A	435	THR
1	A	450	THR
1	A	493	LEU
1	B	4	LEU
1	B	57	SER
1	B	139	ARG
1	B	144	ARG
1	B	183	ASP
1	B	186	ARG
1	B	219	LYS
1	B	236	LYS
1	B	237	TYR
1	B	244	TYR
1	B	276	GLU
1	B	294	GLU
1	B	331	TYR

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Mol	Chain	Res	Type
1	B	332	THR
1	B	421	ARG
1	B	472	ASP
1	B	493	LEU
1	C	3	ASP
1	C	37	SER
1	C	56	SER
1	C	96	ASN
1	C	139	ARG
1	C	144	ARG
1	C	155	GLU
1	C	184	ASN
1	C	219	LYS
1	C	236	LYS
1	C	276	GLU
1	C	280	ASP
1	C	320	SER
1	C	330	ASP
1	C	331	TYR
1	C	380	ASP
1	C	392	VAL
1	C	399	ARG
1	C	421	ARG
1	C	466	ILE
1	C	493	LEU
1	D	96	ASN
1	D	139	ARG
1	D	144	ARG
1	D	199	GLN
1	D	219	LYS
1	D	236	LYS
1	D	237	TYR
1	D	244	TYR
1	D	280	ASP
1	D	306	LYS
1	D	330	ASP
1	D	331	TYR
1	D	332	THR
1	D	371	LYS
1	D	421	ARG
1	D	443	SER
1	D	472	ASP

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Mol	Chain	Res	Type
1	D	477	LEU
1	D	493	LEU
1	E	3	ASP
1	E	40	ASP
1	E	84	SER
1	E	91	ARG
1	E	114	ASP
1	E	115	THR
1	E	139	ARG
1	E	144	ARG
1	E	168	CYS
1	E	219	LYS
1	E	236	LYS
1	E	237	TYR
1	E	262	PHE
1	E	274	THR
1	E	276	GLU
1	E	330	ASP
1	E	331	TYR
1	E	394	MET
1	E	421	ARG
1	E	493	LEU
1	F	1	MET
1	F	3	ASP
1	F	19	TYR
1	F	39	ASN
1	F	61	THR
1	F	91	ARG
1	F	130	ASP
1	F	135	PHE
1	F	139	ARG
1	F	144	ARG
1	F	197	GLU
1	F	199	GLN
1	F	219	LYS
1	F	236	LYS
1	F	237	TYR
1	F	244	TYR
1	F	272	THR
1	F	306	LYS
1	F	330	ASP
1	F	331	TYR

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Mol	Chain	Res	Type
1	F	356	LYS
1	F	394	MET
1	F	399	ARG
1	F	421	ARG
1	F	450	THR
1	F	452	ILE
1	F	472	ASP
1	F	493	LEU
1	G	3	ASP
1	G	37	SER
1	G	45	PRO
1	G	58	SER
1	G	61	THR
1	G	91	ARG
1	G	94	SER
1	G	107	TYR
1	G	115	THR
1	G	135	PHE
1	G	139	ARG
1	G	144	ARG
1	G	168	CYS
1	G	219	LYS
1	G	236	LYS
1	G	237	TYR
1	G	306	LYS
1	G	320	SER
1	G	330	ASP
1	G	331	TYR
1	G	348	LEU
1	G	403	ASN
1	G	419	THR
1	G	421	ARG
1	G	430	PHE
1	G	462	GLU
1	G	477	LEU
1	G	493	LEU
1	H	3	ASP
1	H	58	SER
1	H	84	SER
1	H	91	ARG
1	H	96	ASN
1	H	107	TYR

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Mol	Chain	Res	Type
1	H	114	ASP
1	H	115	THR
1	H	117	ASP
1	H	119	ASP
1	H	139	ARG
1	H	144	ARG
1	H	219	LYS
1	H	236	LYS
1	H	237	TYR
1	H	244	TYR
1	H	245	SER
1	H	262	PHE
1	H	331	TYR
1	H	371	LYS
1	H	421	ARG
1	H	443	SER
1	H	476	ASP
1	H	493	LEU
1	I	36	ASP
1	I	139	ARG
1	I	144	ARG
1	I	219	LYS
1	I	228	GLU
1	I	236	LYS
1	I	237	TYR
1	I	273	THR
1	I	330	ASP
1	I	331	TYR
1	I	373	ASP
1	I	394	MET
1	I	403	ASN
1	I	421	ARG
1	I	450	THR
1	I	493	LEU
1	J	3	ASP
1	J	40	ASP
1	J	56	SER
1	J	73	CYS
1	J	84	SER
1	J	98	LYS
1	J	114	ASP
1	J	115	THR

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Mol	Chain	Res	Type
1	J	122	ASN
1	J	130	ASP
1	J	132	GLU
1	J	139	ARG
1	J	144	ARG
1	J	168	CYS
1	J	219	LYS
1	J	236	LYS
1	J	237	TYR
1	J	272	THR
1	J	330	ASP
1	J	331	TYR
1	J	421	ARG
1	J	450	THR
1	J	476	ASP
1	J	477	LEU
1	J	493	LEU
1	K	3	ASP
1	K	32	SER
1	K	91	ARG
1	K	107	TYR
1	K	114	ASP
1	K	139	ARG
1	K	144	ARG
1	K	194	ASP
1	K	197	GLU
1	K	219	LYS
1	K	236	LYS
1	K	237	TYR
1	K	244	TYR
1	K	330	ASP
1	K	331	TYR
1	K	357	GLU
1	K	373	ASP
1	K	403	ASN
1	K	419	THR
1	K	421	ARG
1	K	443	SER
1	K	450	THR
1	K	477	LEU
1	K	493	LEU
1	L	1	MET

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Mol	Chain	Res	Type
1	L	3	ASP
1	L	19	TYR
1	L	29	GLN
1	L	58	SER
1	L	91	ARG
1	L	98	LYS
1	L	114	ASP
1	L	115	THR
1	L	139	ARG
1	L	144	ARG
1	L	219	LYS
1	L	236	LYS
1	L	237	TYR
1	L	331	TYR
1	L	392	VAL
1	L	396	ASN
1	L	421	ARG
1	L	472	ASP
1	L	493	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	B	108	ASN
1	B	124	ASN
1	B	403	ASN
1	D	106	GLN
1	D	137	HIS
1	D	382	GLN
1	E	16	GLN
1	E	184	ASN
1	E	267	ASN
1	G	30	GLN
1	G	137	HIS
1	I	184	ASN
1	J	137	HIS
1	J	177	GLN
1	J	207	ASN
1	J	403	ASN
1	K	133	HIS
1	K	137	HIS

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Mol	Chain	Res	Type
1	K	199	GLN
1	L	177	GLN
1	L	283	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 12 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	C	501	-	5,5,5	0.18	0	5,5,5	0.43	0

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	GOL	C	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	GOL	O1-C1-C2-O2
3	C	501	GOL	O1-C1-C2-C3

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 [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	491/496 (98%)	-0.48	2 (0%) 92 87	56, 102, 159, 278	0
1	B	494/496 (99%)	-0.34	5 (1%) 82 71	70, 113, 180, 228	0
1	C	487/496 (98%)	-0.36	3 (0%) 89 81	65, 108, 171, 216	0
1	D	495/496 (99%)	-0.30	7 (1%) 75 62	64, 112, 191, 271	0
1	E	495/496 (99%)	-0.34	13 (2%) 56 42	60, 111, 179, 213	0
1	F	495/496 (99%)	-0.48	2 (0%) 92 87	49, 102, 158, 222	0
1	G	495/496 (99%)	-0.31	8 (1%) 72 59	49, 105, 199, 283	0
1	H	495/496 (99%)	-0.37	6 (1%) 79 67	64, 114, 171, 207	0
1	I	495/496 (99%)	-0.24	10 (2%) 65 52	68, 118, 184, 296	0
1	J	495/496 (99%)	-0.29	4 (0%) 86 75	68, 115, 184, 241	0
1	K	495/496 (99%)	-0.35	3 (0%) 89 81	67, 115, 188, 236	0
1	L	495/496 (99%)	-0.23	9 (1%) 68 54	67, 121, 184, 243	0
All	All	5927/5952 (99%)	-0.34	72 (1%) 79 67	49, 111, 181, 296	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	240	PRO	12.3
1	I	239	MET	6.2
1	G	240	PRO	5.6
1	I	418	PRO	5.0
1	L	380	ASP	4.3
1	G	241	GLU	4.0
1	B	240	PRO	3.4
1	I	241	GLU	3.4
1	J	242	ASP	3.3
1	K	234	ARG	3.3
1	D	365	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	365	PRO	3.3
1	L	244	TYR	3.3
1	L	418	PRO	3.3
1	E	369	GLY	3.2
1	A	380	ASP	3.2
1	C	242	ASP	3.1
1	E	367	SER	3.1
1	D	37	SER	3.0
1	E	372	ALA	3.0
1	A	381	GLY	3.0
1	C	378	VAL	3.0
1	I	349	GLU	2.9
1	D	373	ASP	2.9
1	L	242	ASP	2.9
1	G	352	PRO	2.8
1	D	234	ARG	2.8
1	L	347	MET	2.8
1	H	3	ASP	2.8
1	E	368	ILE	2.7
1	F	365	PRO	2.7
1	G	249	ILE	2.6
1	H	242	ASP	2.6
1	B	242	ASP	2.6
1	H	1	MET	2.6
1	I	244	TYR	2.6
1	E	373	ASP	2.6
1	L	364	HIS	2.6
1	G	282	PRO	2.5
1	E	347	MET	2.5
1	J	240	PRO	2.5
1	D	219	LYS	2.5
1	K	415	PRO	2.5
1	J	241	GLU	2.4
1	E	381	GLY	2.4
1	C	373	ASP	2.4
1	B	372	ALA	2.4
1	K	118	MET	2.4
1	I	411	GLU	2.3
1	E	374	PRO	2.3
1	G	373	ASP	2.3
1	I	419	THR	2.3
1	L	241	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	418	PRO	2.2
1	B	373	ASP	2.2
1	G	250	ARG	2.2
1	E	247	LYS	2.2
1	E	285	PRO	2.2
1	D	230	LEU	2.1
1	E	240	PRO	2.1
1	I	367	SER	2.1
1	B	250	ARG	2.1
1	D	237	TYR	2.1
1	L	349	GLU	2.1
1	H	365	PRO	2.1
1	J	227	GLU	2.1
1	E	366	LEU	2.1
1	H	348	LEU	2.0
1	L	346	HIS	2.0
1	F	349	GLU	2.0
1	H	367	SER	2.0
1	I	321	LEU	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
2	MN	D	501	1/1	0.71	0.17	135,135,135,135	0
2	MN	I	501	1/1	0.88	0.08	112,112,112,112	0
2	MN	J	501	1/1	0.89	0.10	115,115,115,115	0
3	GOL	C	501	6/6	0.92	0.21	76,89,94,107	0

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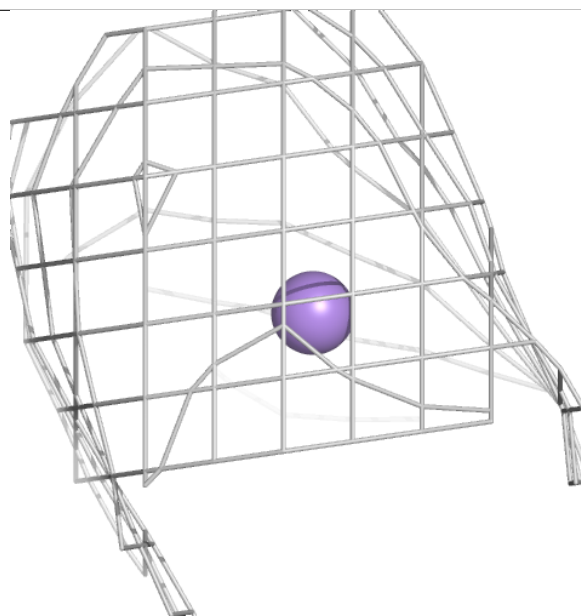
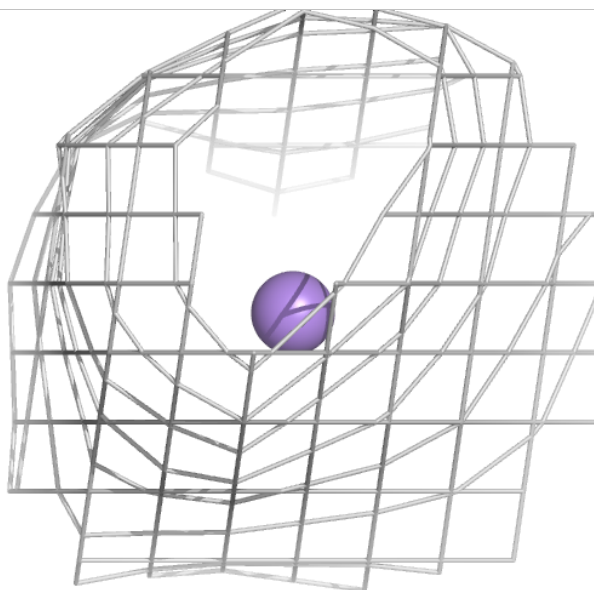
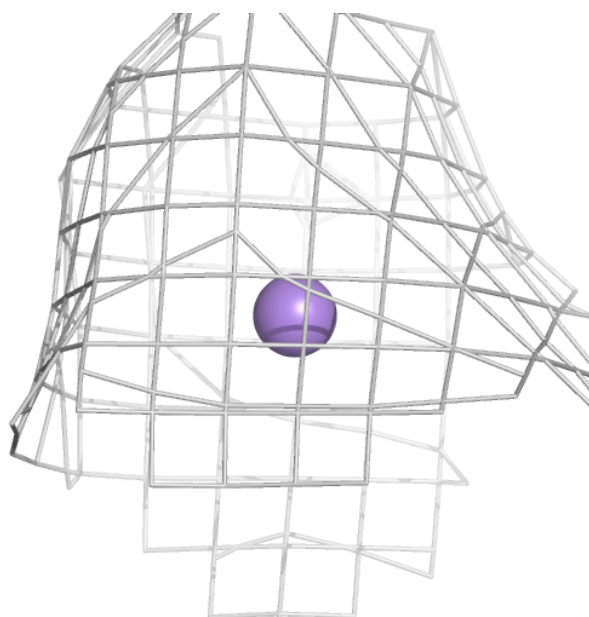
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	E	501	1/1	0.93	0.06	115,115,115,115	0
2	MN	H	501	1/1	0.94	0.08	109,109,109,109	0
2	MN	G	501	1/1	0.94	0.10	99,99,99,99	0
2	MN	B	501	1/1	0.95	0.09	112,112,112,112	0
2	MN	K	501	1/1	0.96	0.12	117,117,117,117	0
2	MN	F	501	1/1	0.96	0.07	84,84,84,84	0
2	MN	L	501	1/1	0.98	0.04	85,85,85,85	0
2	MN	C	502	1/1	0.99	0.08	112,112,112,112	0
2	MN	A	501	1/1	1.00	0.06	84,84,84,84	0

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

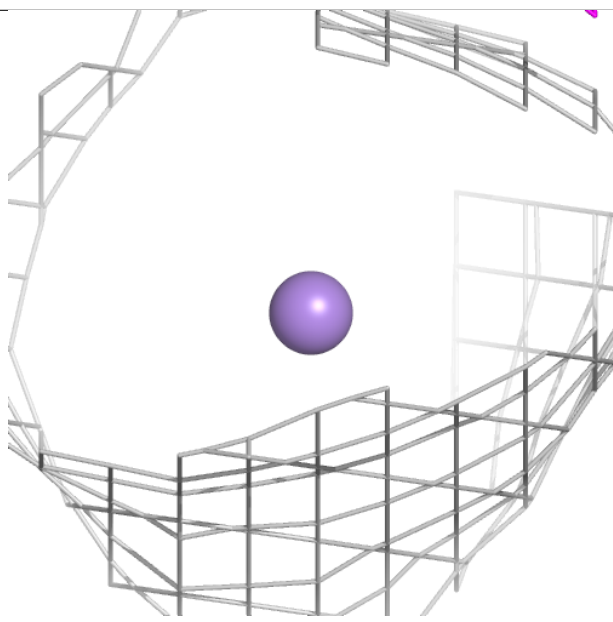
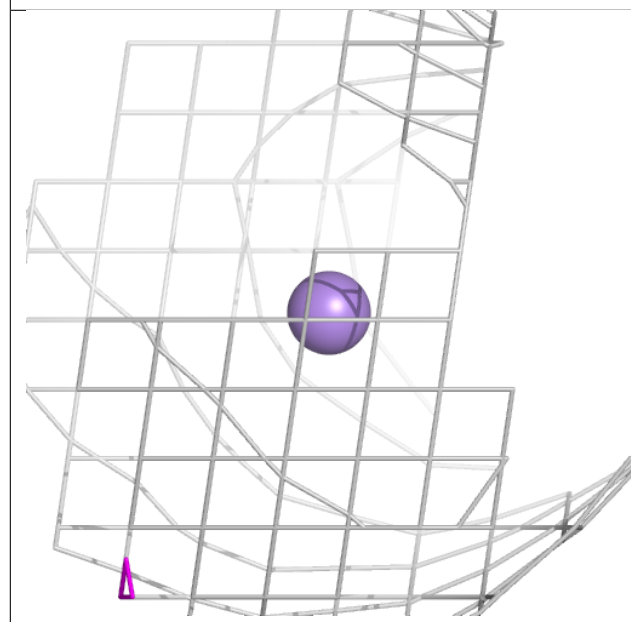
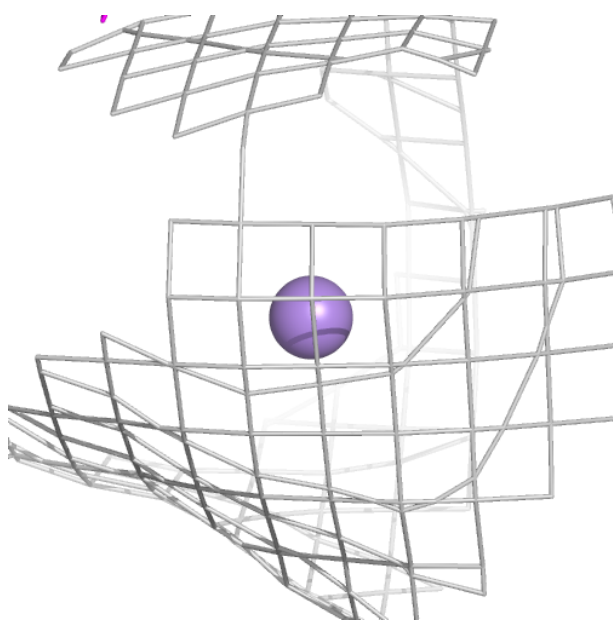
Electron density around MN D 501:

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



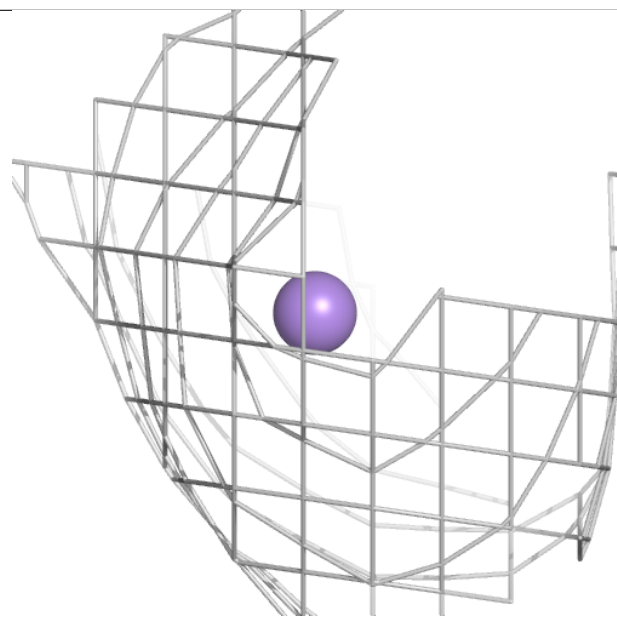
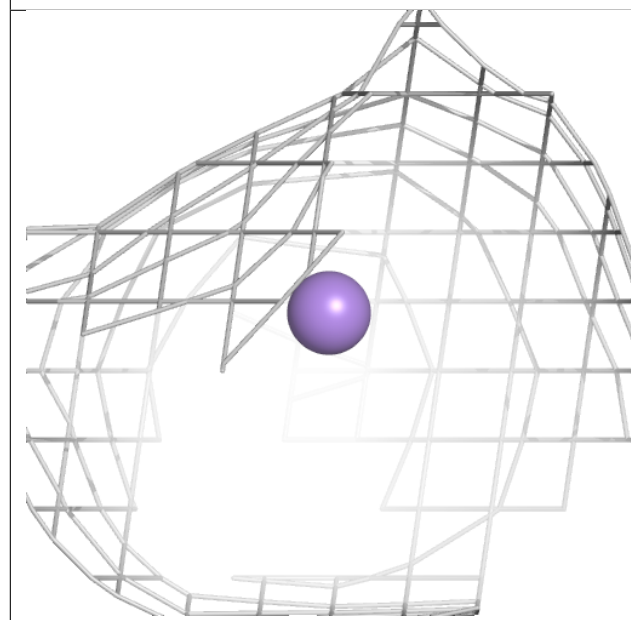
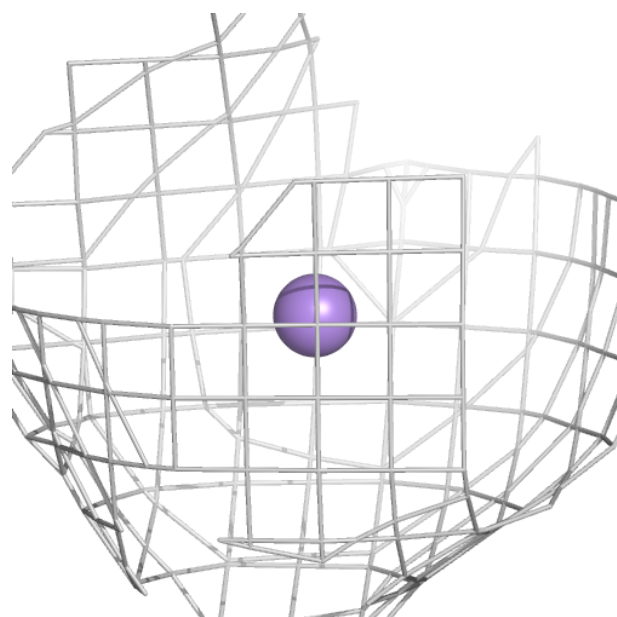
Electron density around MN I 501:

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



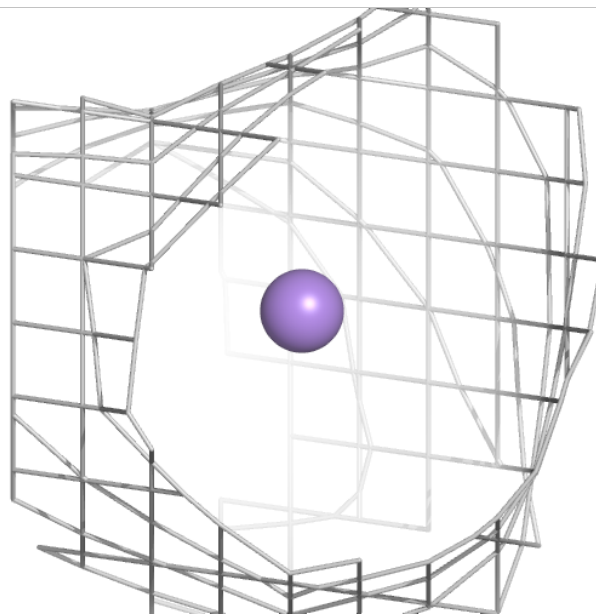
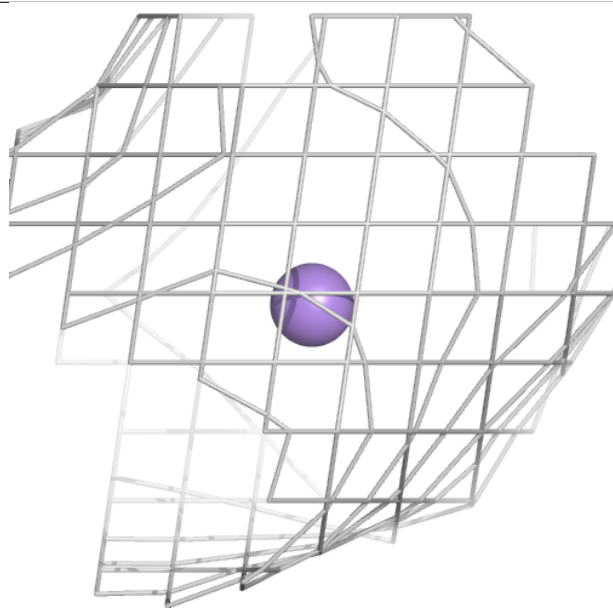
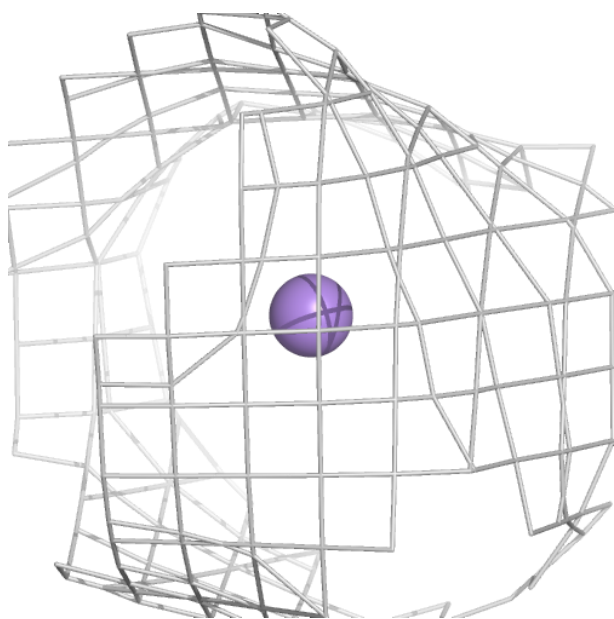
Electron density around MN J 501:

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



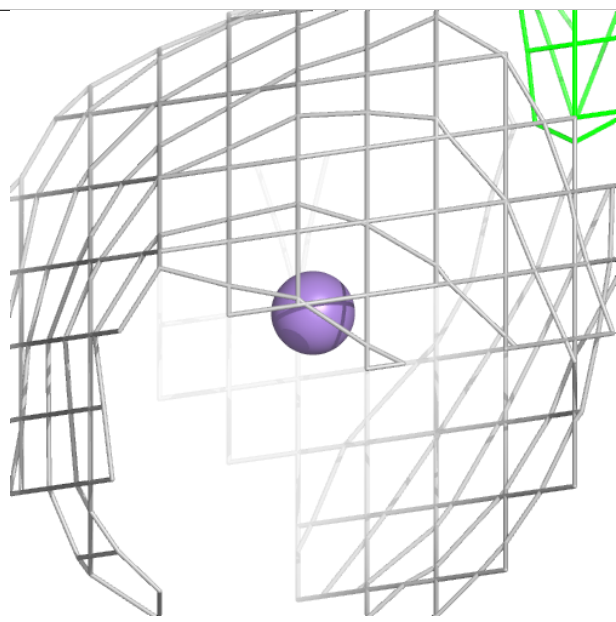
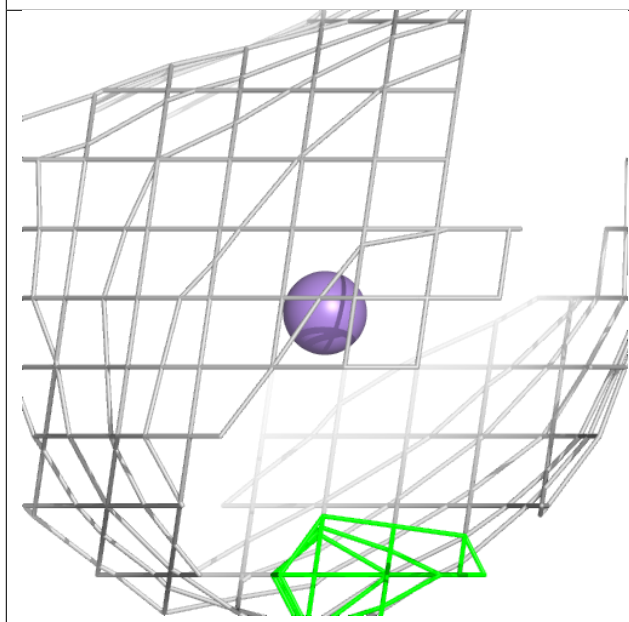
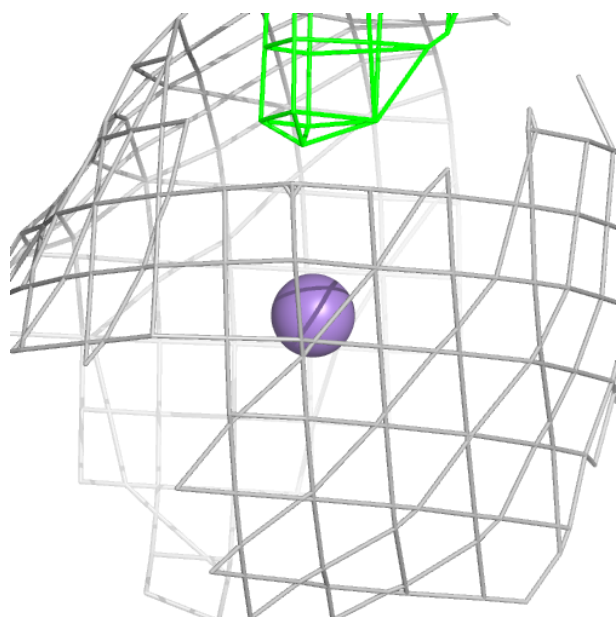
Electron density around MN E 501:

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



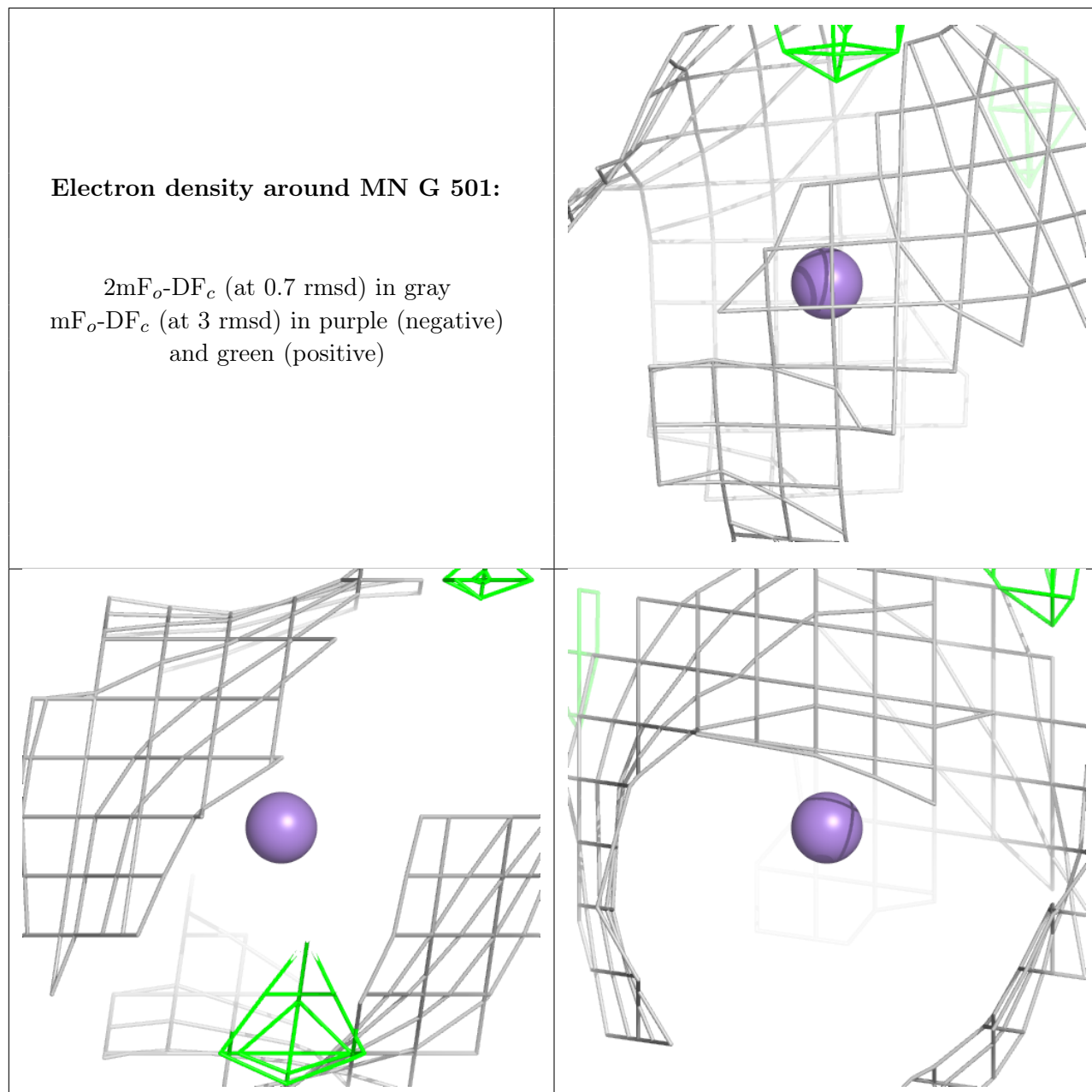
Electron density around MN H 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



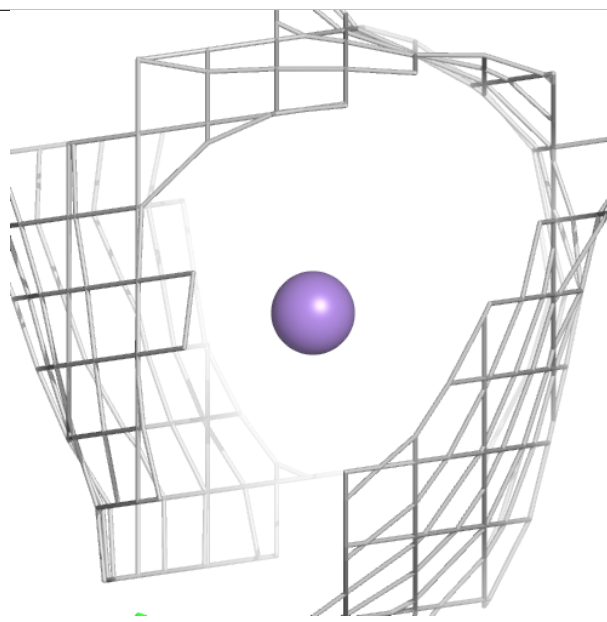
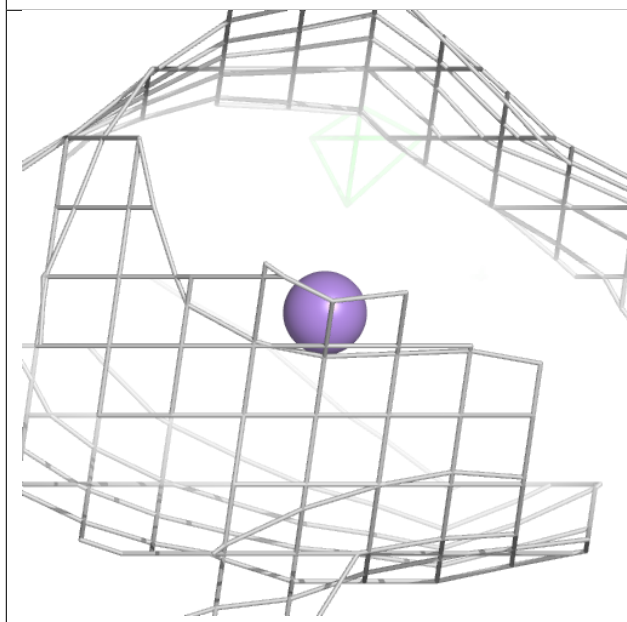
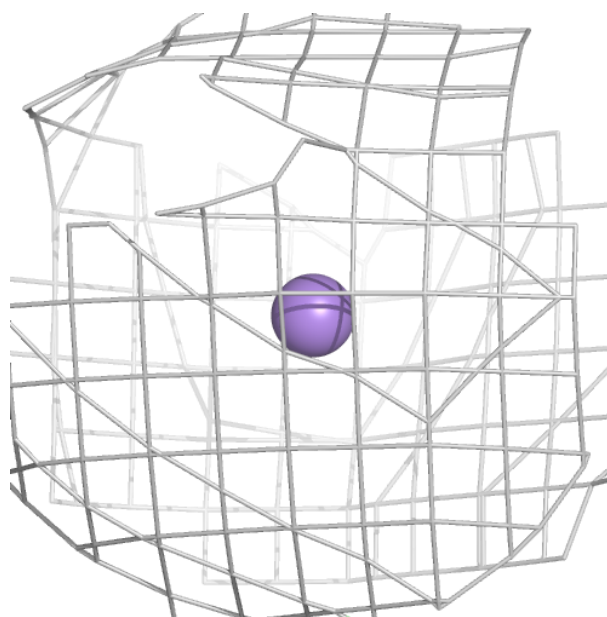
Electron density around MN G 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



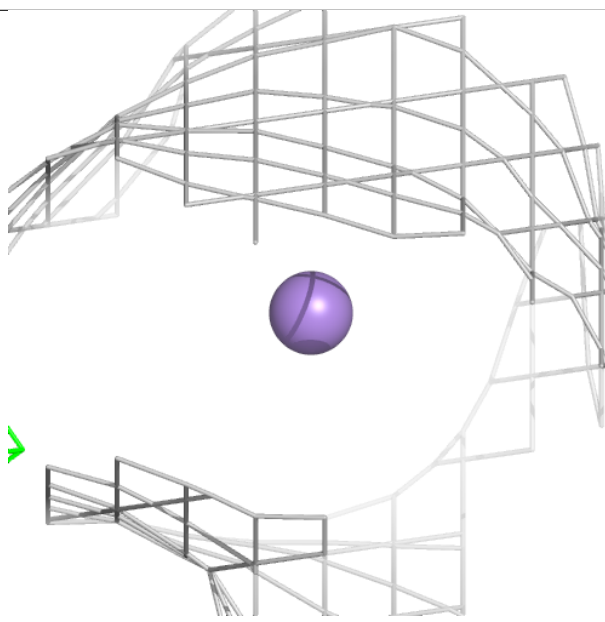
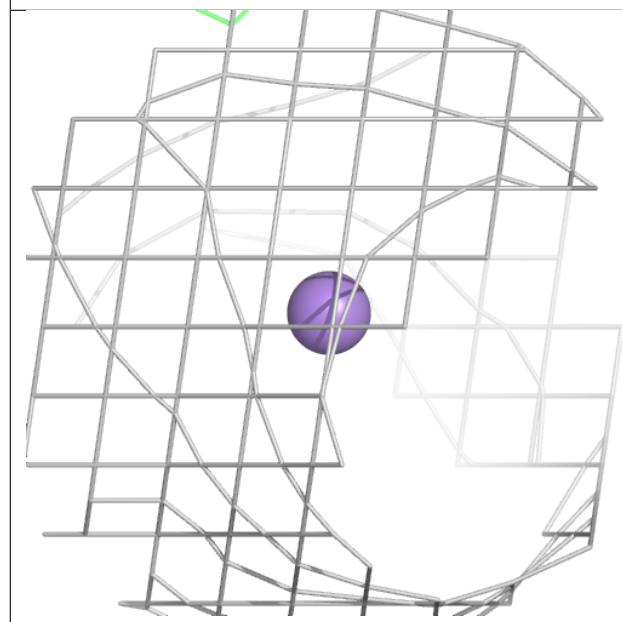
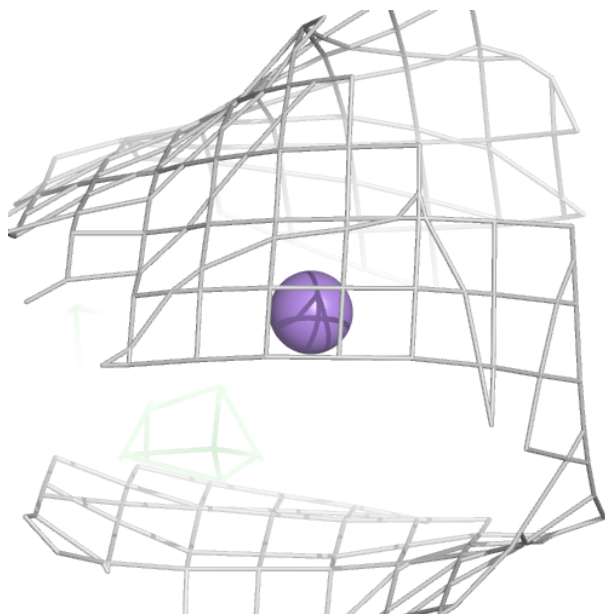
Electron density around MN B 501:

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and green (positive)



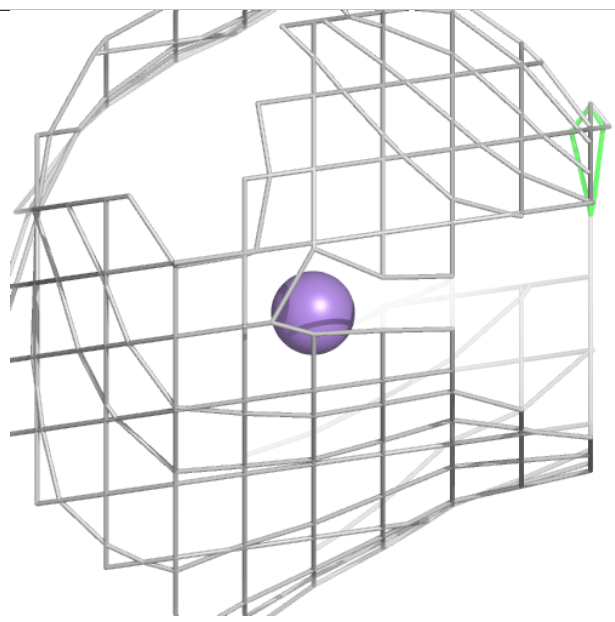
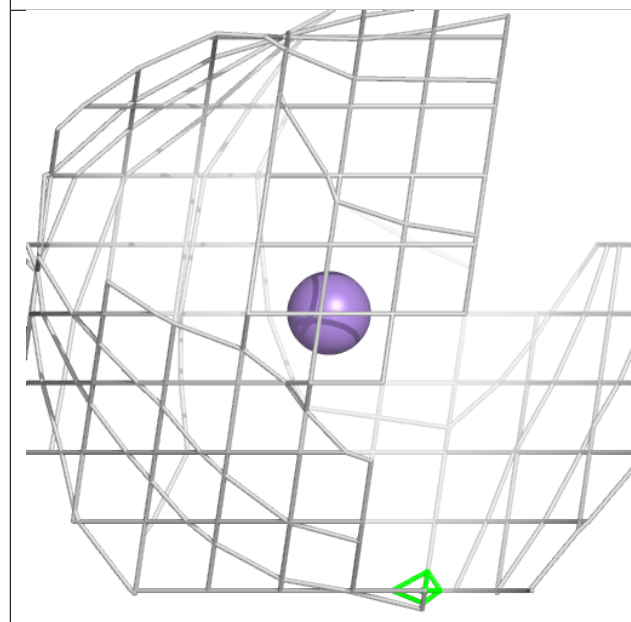
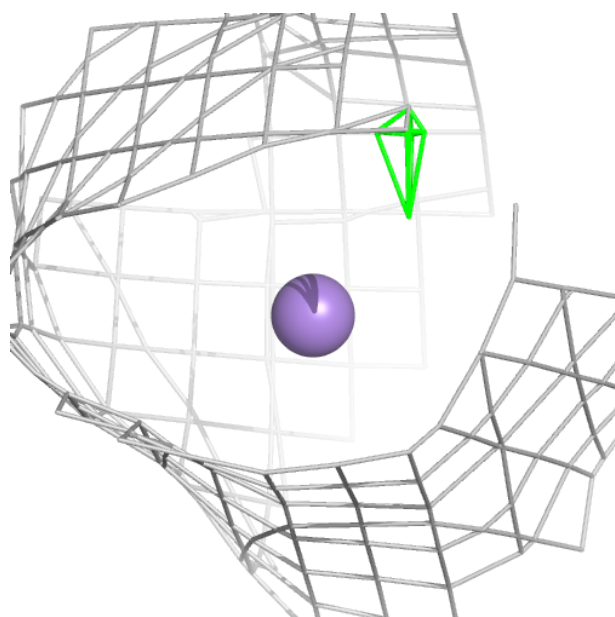
Electron density around MN K 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



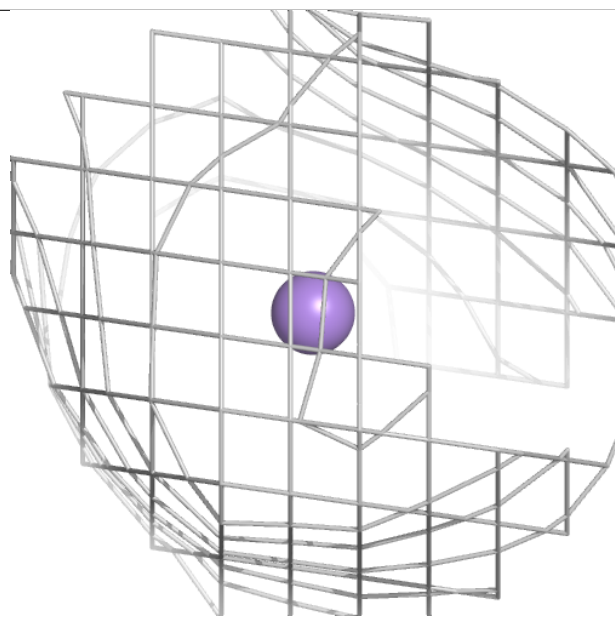
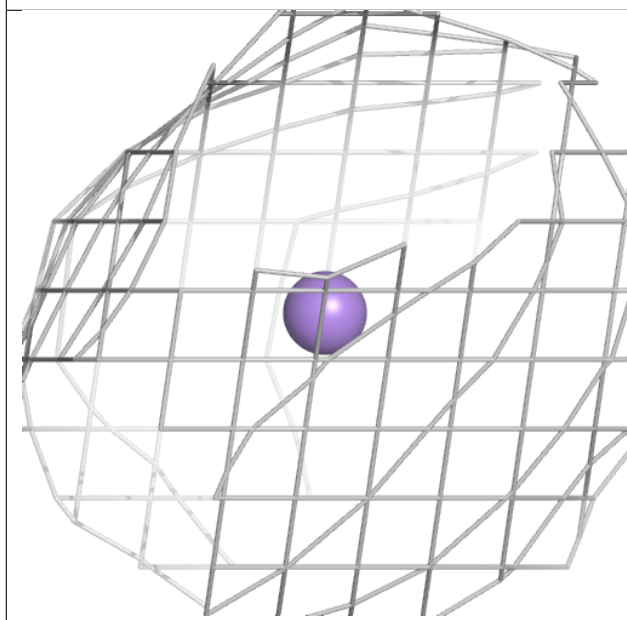
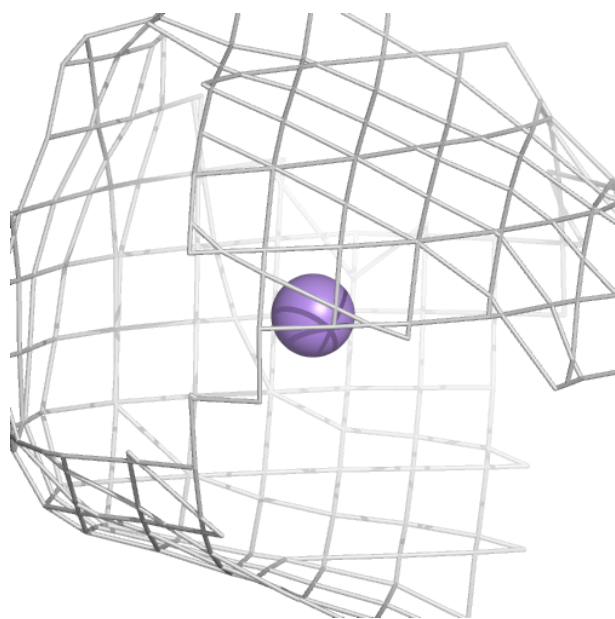
Electron density around MN F 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



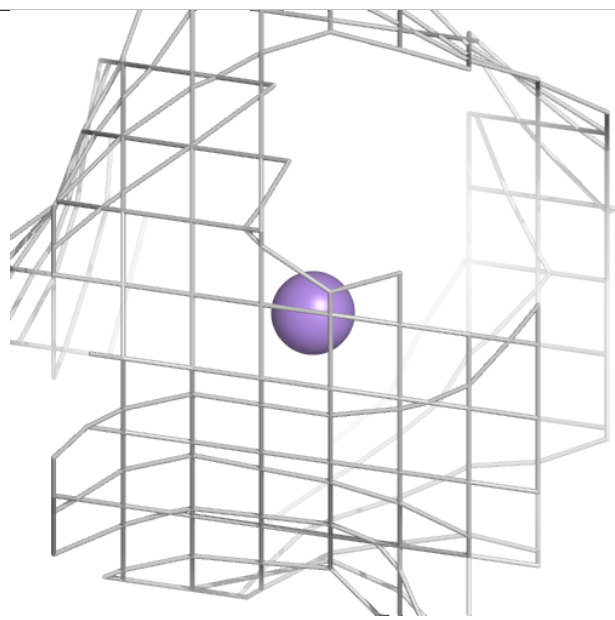
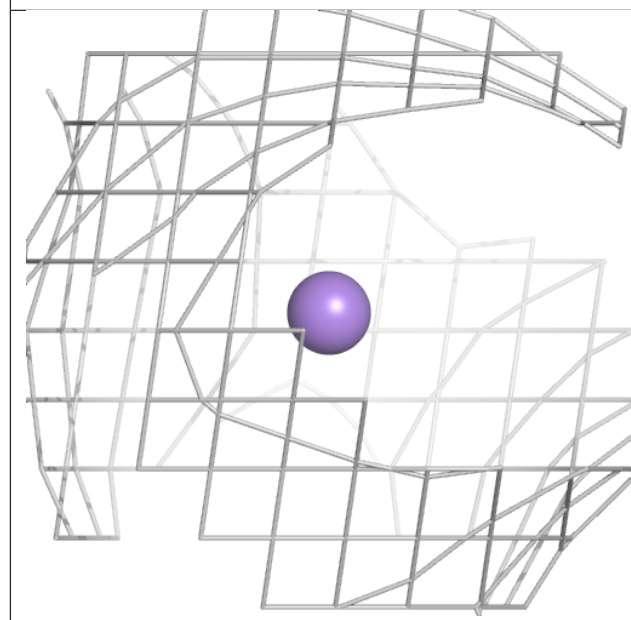
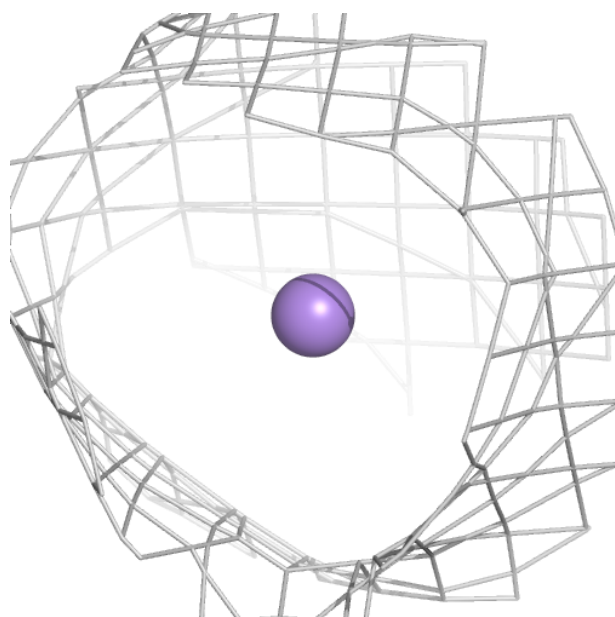
Electron density around MN L 501:

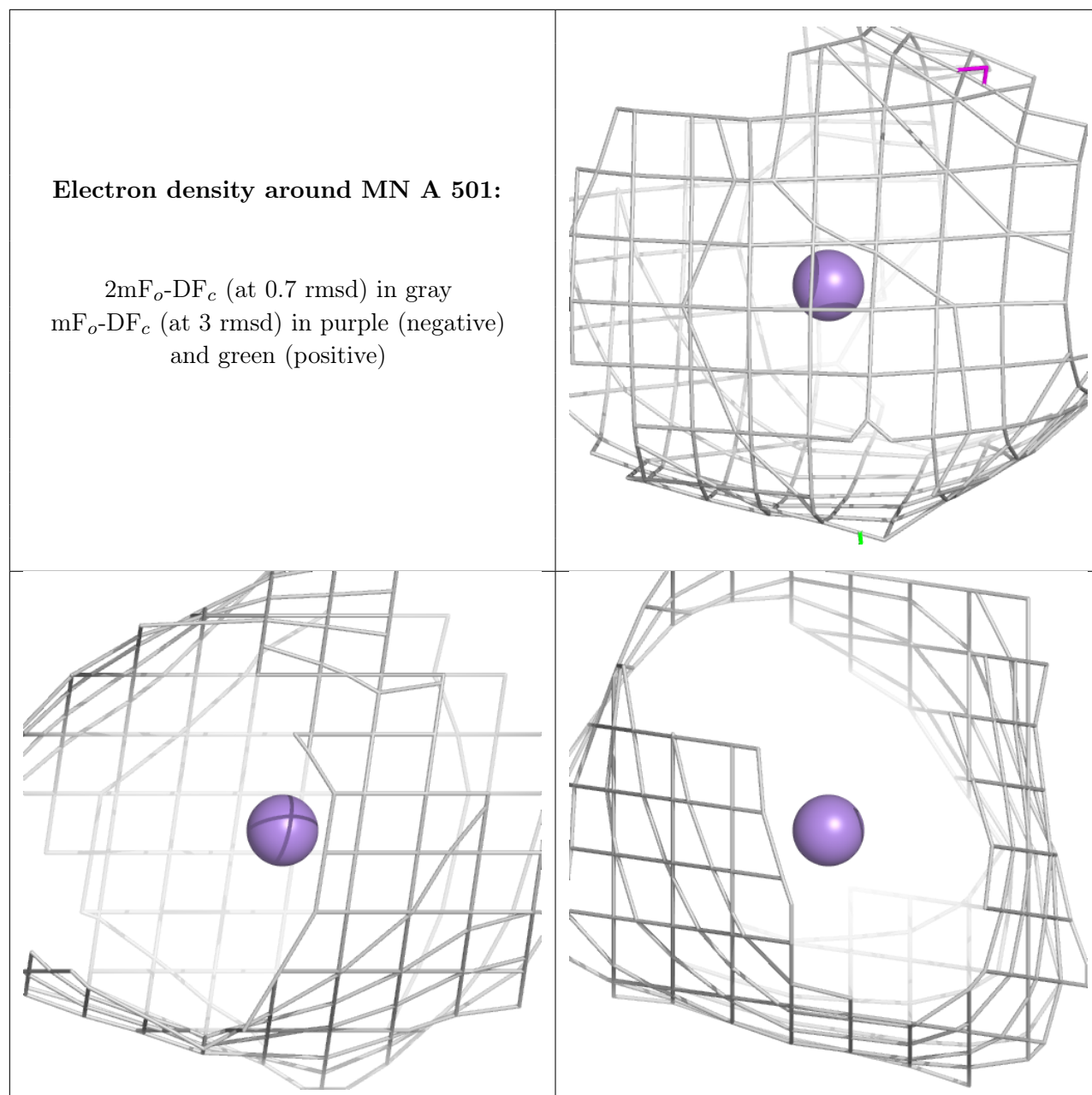
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN C 502:

$2mF_o-DF_c$ (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.