



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:39 PM EDT

PDB ID : 8JIB / pdb_00008jib
Title : Crystal Structure of Prophenoloxidase PPO6 from Aedes aegypti
Authors : Zhu, X.; Zhang, L.; Yang, X.; Bao, P.; Ren, D.; Han, Q.
Deposited on : 2023-05-26
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

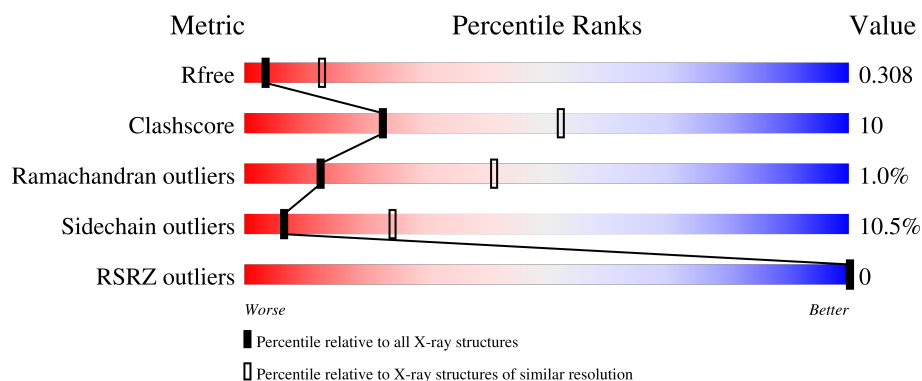
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	681	
1	B	681	
1	C	681	
1	D	681	
1	E	681	

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Mol	Chain	Length	Quality of chain
1	F	681	72% 19% 6%
1	G	681	75% 17%
1	H	681	74% 19%
1	I	681	73% 20%
1	J	681	73% 20%
1	K	681	75% 18%
1	L	681	74% 18%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 65153 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 TK receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5377	3422	969	961	25			
1	B	645	Total	C	N	O	S	0	0	0
			5330	3395	960	952	23			
1	C	648	Total	C	N	O	S	0	0	0
			5358	3412	966	955	25			
1	D	650	Total	C	N	O	S	0	0	0
			5373	3420	968	960	25			
1	E	661	Total	C	N	O	S	0	0	0
			5450	3466	981	976	27			
1	F	657	Total	C	N	O	S	0	0	0
			5421	3448	976	971	26			
1	G	659	Total	C	N	O	S	0	0	0
			5431	3453	978	973	27			
1	H	661	Total	C	N	O	S	0	0	0
			5450	3466	981	976	27			
1	I	660	Total	C	N	O	S	0	0	0
			5442	3462	979	974	27			
1	J	659	Total	C	N	O	S	0	0	0
			5431	3453	978	973	27			
1	K	660	Total	C	N	O	S	0	0	0
			5442	3462	979	974	27			
1	L	659	Total	C	N	O	S	0	0	0
			5431	3453	978	973	27			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

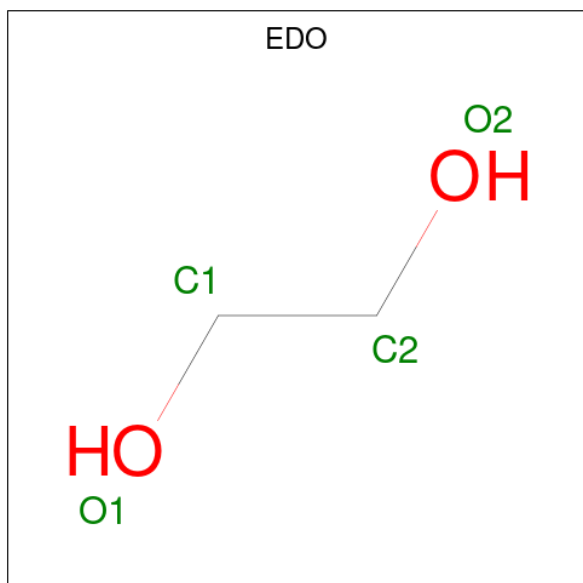
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

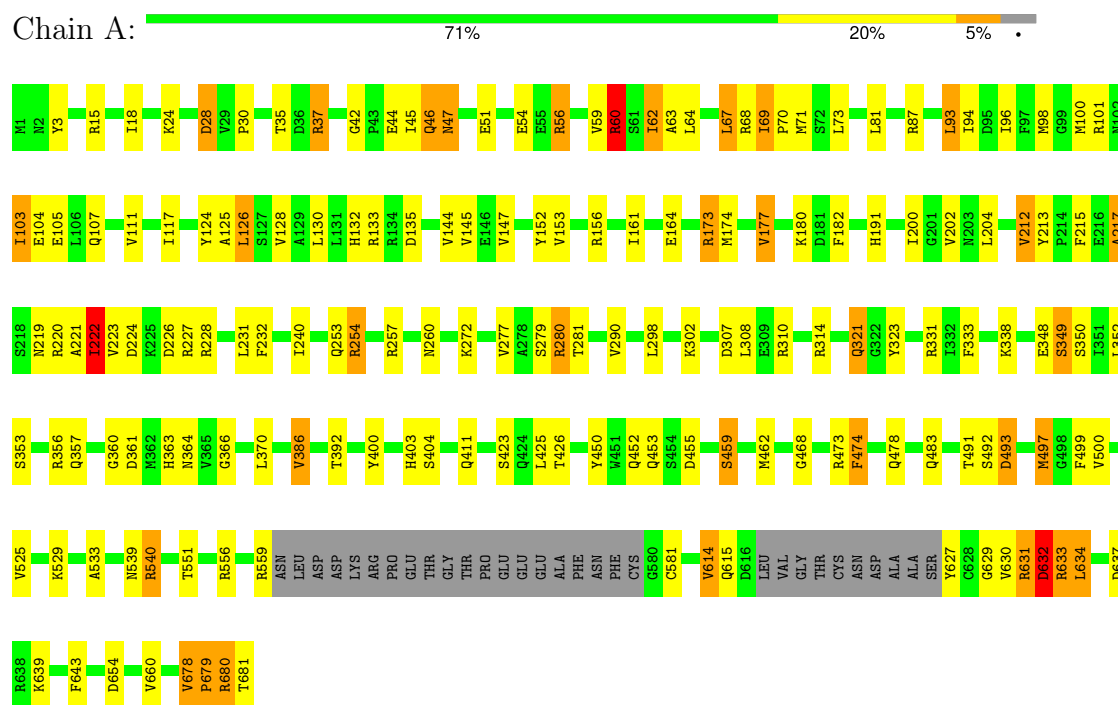
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	25	Total	O	0	0
			25	25		
4	C	23	Total	O	0	0
			23	23		
4	D	13	Total	O	0	0
			13	13		
4	E	14	Total	O	0	0
			14	14		
4	F	12	Total	O	0	0
			12	12		
4	G	8	Total	O	0	0
			8	8		
4	H	6	Total	O	0	0
			6	6		
4	I	8	Total	O	0	0
			8	8		
4	J	6	Total	O	0	0
			6	6		
4	K	1	Total	O	0	0
			1	1		
4	L	18	Total	O	0	0
			18	18		

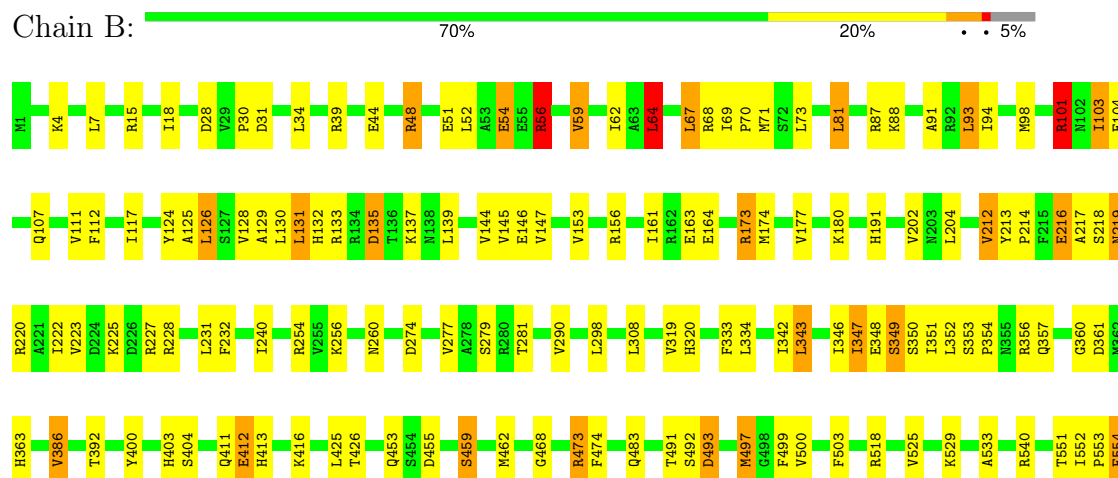
3 Residue-property plots

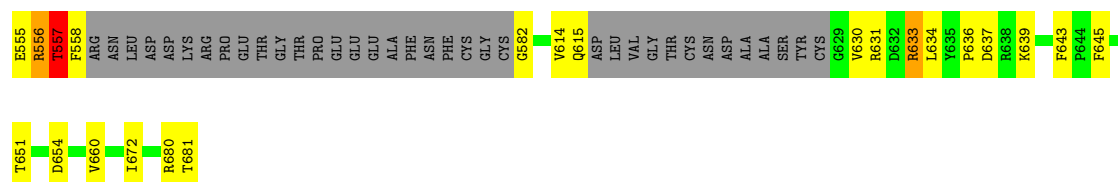
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



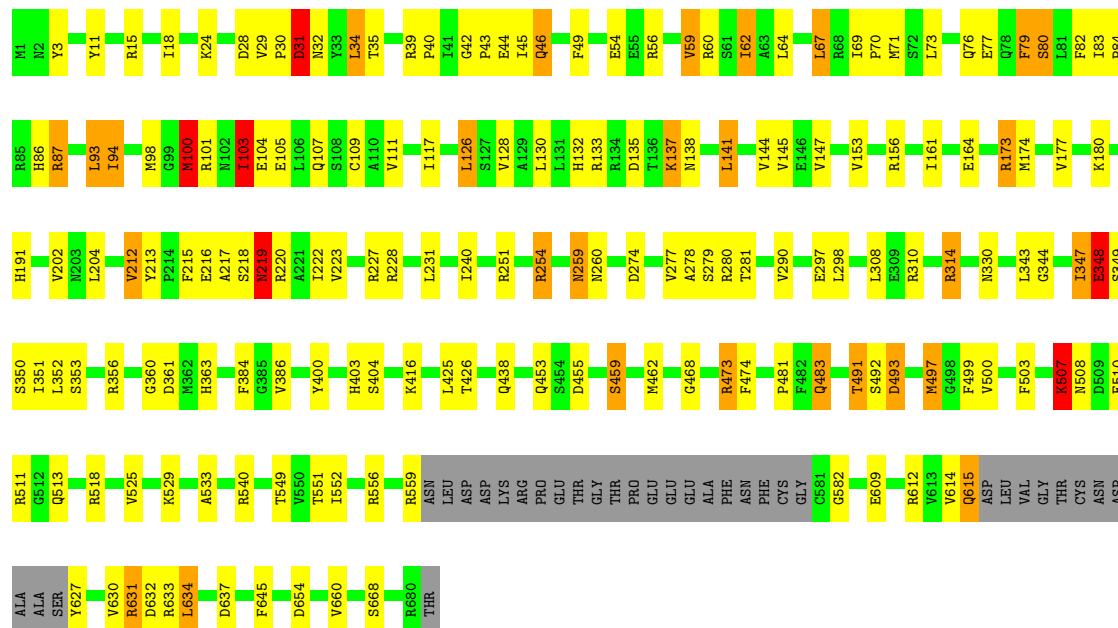
• Molecule 1: TK receptor





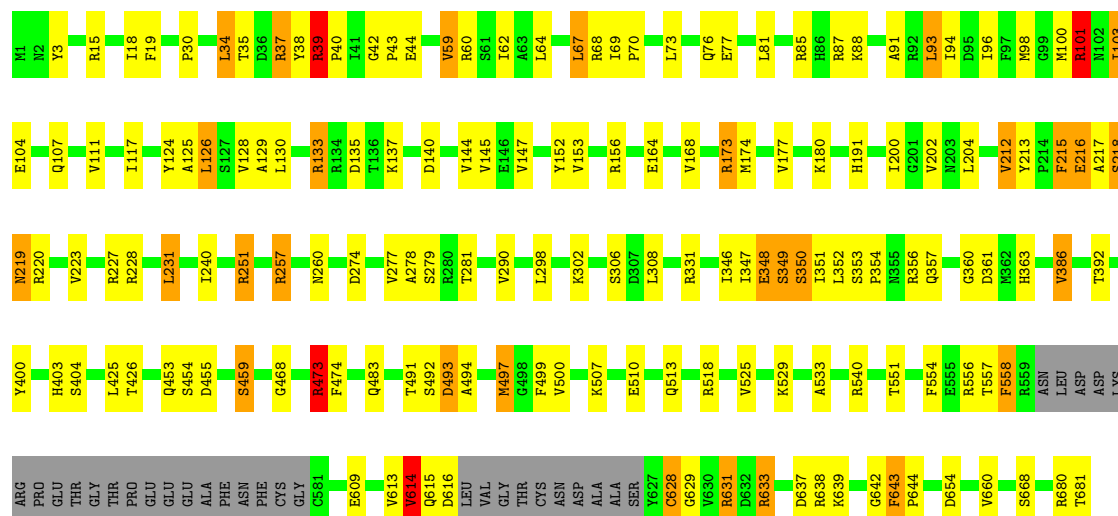
• Molecule 1: TK receptor

Chain C: 69% 21% 5%



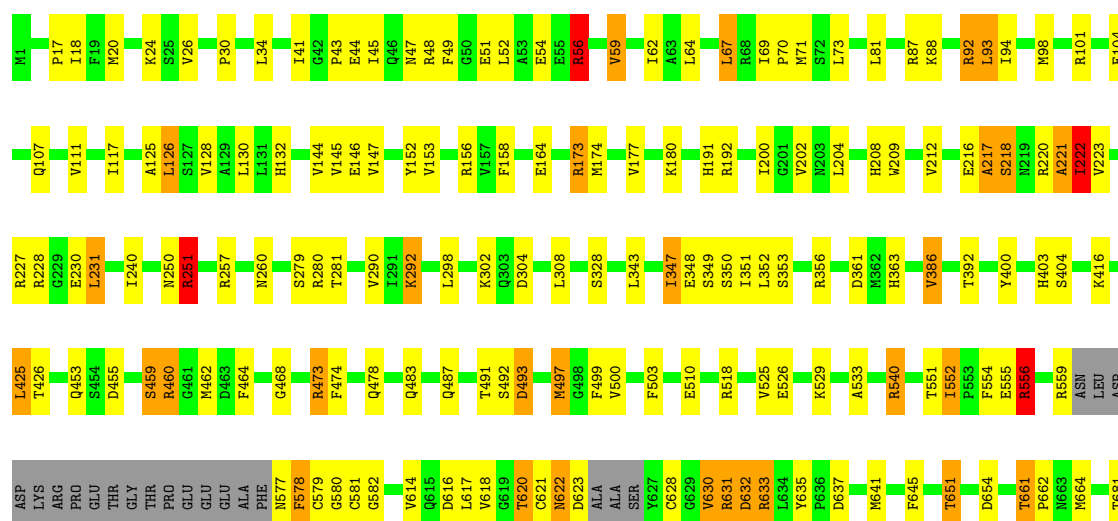
• Molecule 1: TK receptor

Chain D: 72% 19% 5%



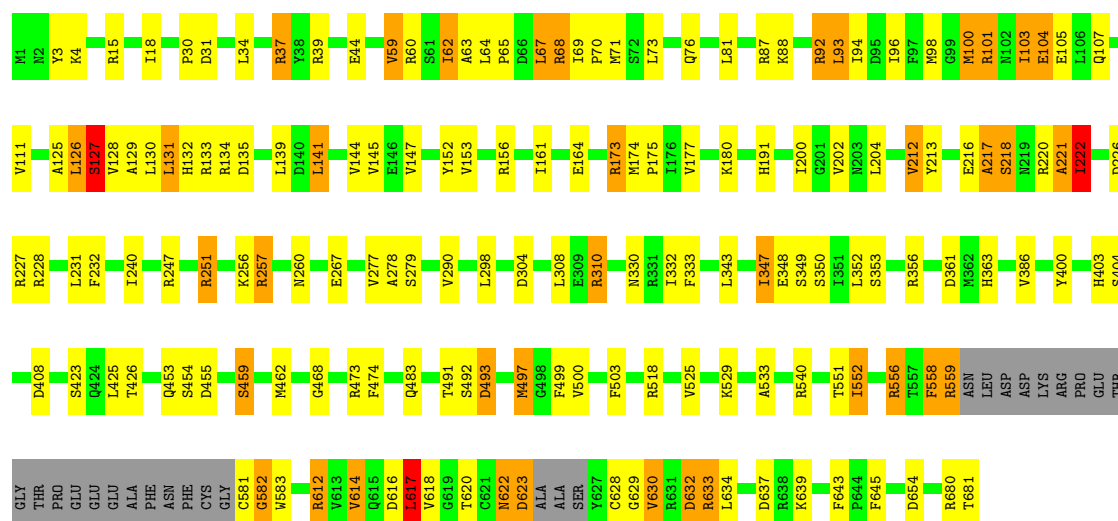
• Molecule 1: TK receptor

Chain E:  72% 20% . . .



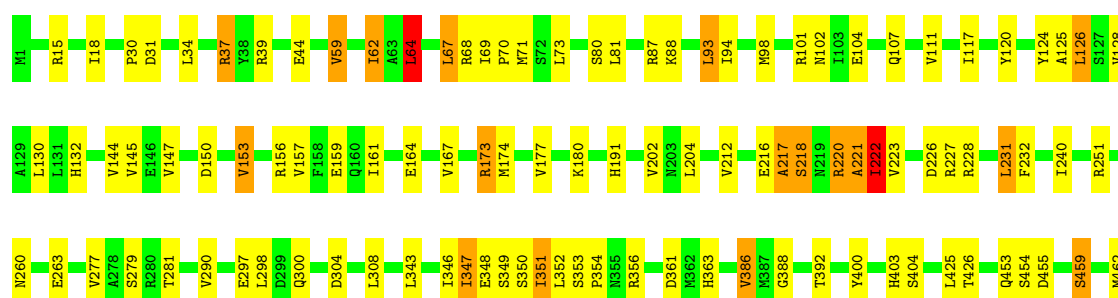
• Molecule 1: TK receptor

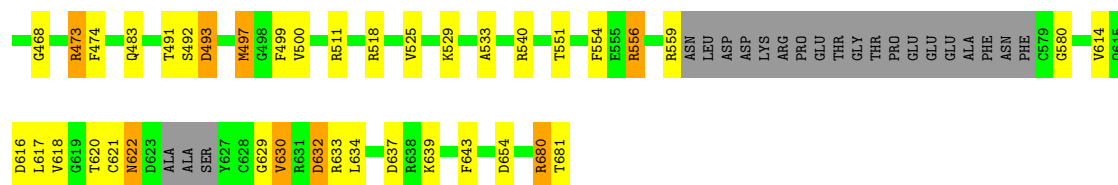
Chain F:  72% 19% 6% .



• Molecule 1: TK receptor

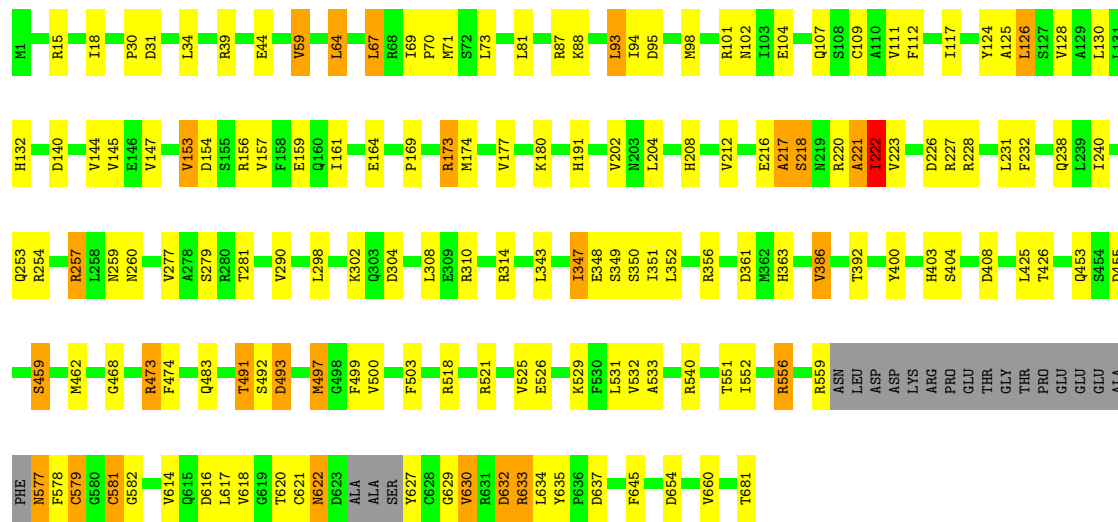
Chain G:  75% 17% . . .





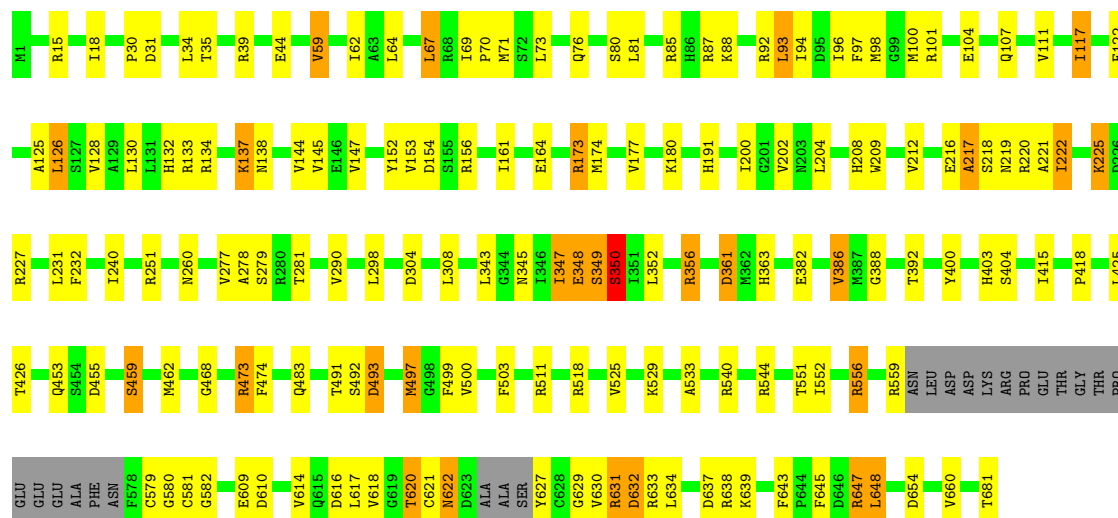
• Molecule 1: TK receptor

Chain H: 74% 19%



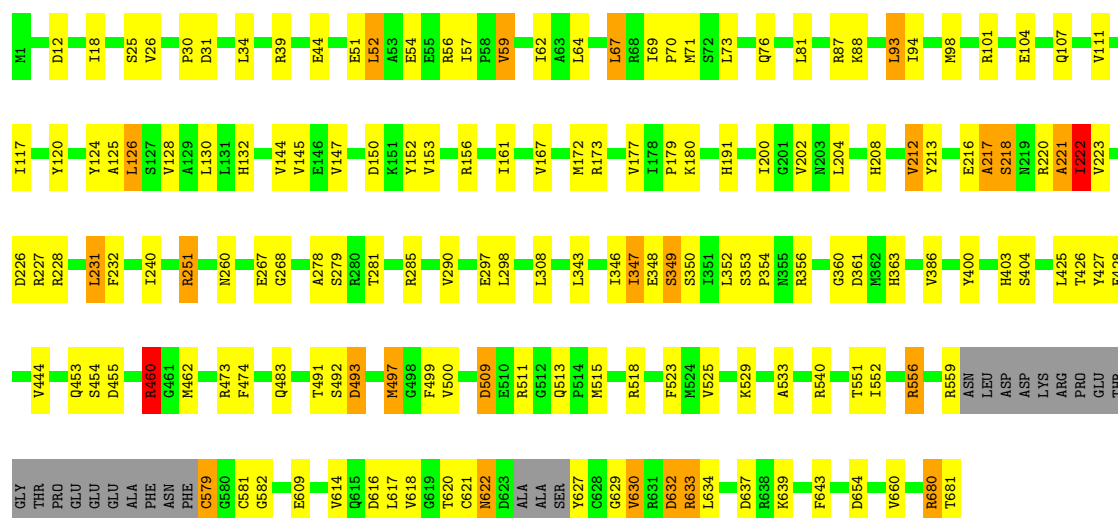
• Molecule 1: TK receptor

Chain I: 73% 20%



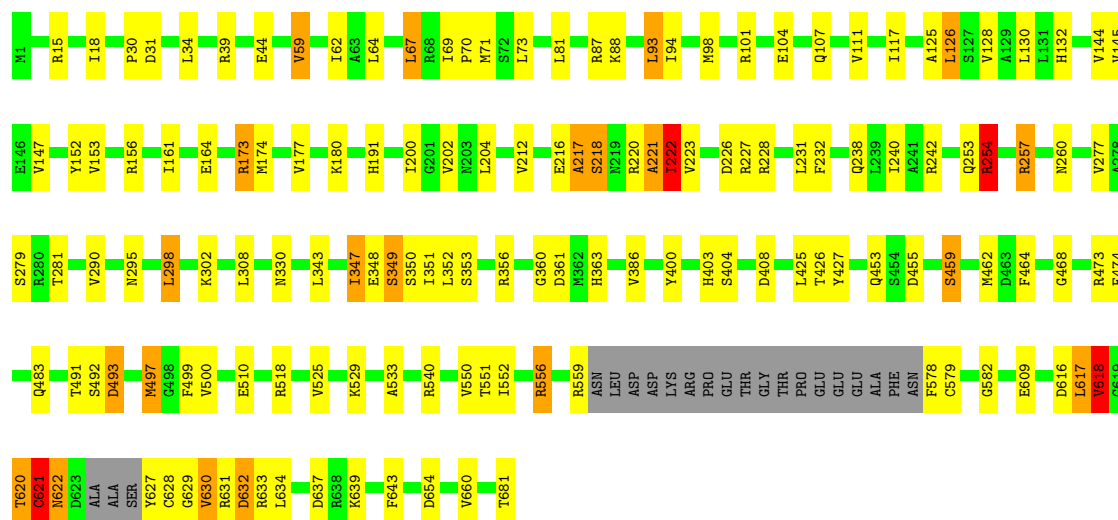
• Molecule 1: TK receptor

Chain J: 73% 20%



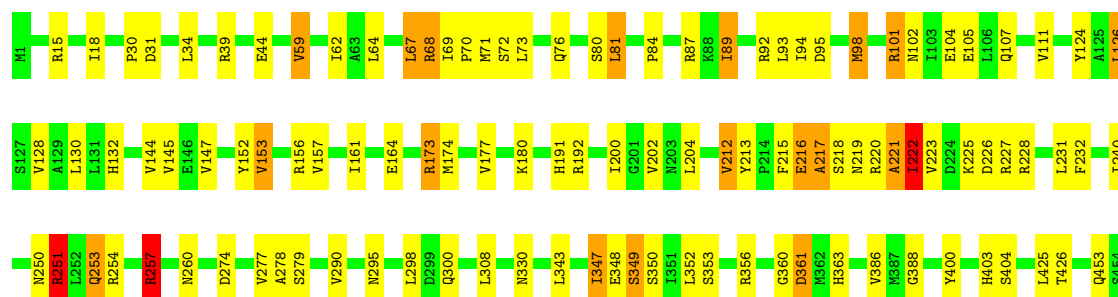
• Molecule 1: TK receptor

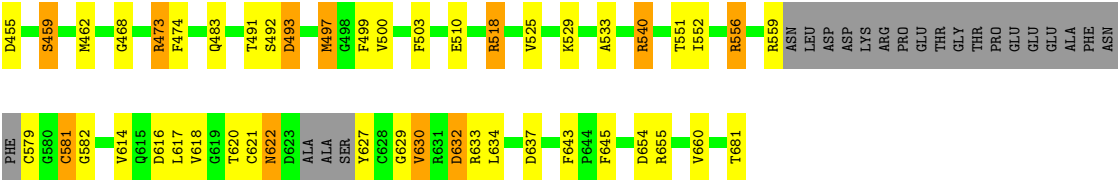
Chain K: 75% 18%



• Molecule 1: TK receptor

Chain L: 74% 18%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.04Å 364.15Å 125.52Å 90.00° 118.95° 90.00°	Depositor
Resolution (Å)	48.66 – 3.15 48.66 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.66-3.15) 98.2 (48.66-3.15)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.269 , 0.310 0.269 , 0.308	Depositor DCC
R_{free} test set	7921 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.046 for l,k,-h-l 0.046 for -h-l,k,h 0.387 for h,-k,-h-l 0.047 for l,-k,h 0.047 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	65153	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.38% 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: EDO, CU

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	0.55	0/5513	1.07	10/7461 (0.1%)
1	B	0.54	0/5465	1.03	5/7397 (0.1%)
1	C	0.54	0/5494	1.06	15/7435 (0.2%)
1	D	0.57	0/5509	1.04	9/7456 (0.1%)
1	E	0.53	0/5587	1.02	6/7562 (0.1%)
1	F	0.53	0/5557	1.05	12/7522 (0.2%)
1	G	0.51	0/5567	0.98	1/7535 (0.0%)
1	H	0.51	0/5587	0.99	3/7562 (0.0%)
1	I	0.52	0/5579	1.01	8/7551 (0.1%)
1	J	0.51	0/5567	1.00	4/7535 (0.1%)
1	K	0.50	0/5579	0.98	4/7551 (0.1%)
1	L	0.51	0/5567	0.99	7/7535 (0.1%)
All	All	0.53	0/66571	1.02	84/90102 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	3
1	E	0	3
1	F	0	4
1	G	0	1
1	H	0	2
1	J	0	2
1	K	0	1
1	L	0	2
All	All	0	20

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	PHE	CB-CA-C	10.70	131.72	110.42
1	F	228	ARG	CG-CD-NE	-9.28	91.59	112.00
1	F	247	ARG	CG-CD-NE	-9.01	92.18	112.00
1	K	620	THR	CA-CB-OG1	-8.39	97.01	109.60
1	H	408	ASP	CA-CB-CG	7.70	120.30	112.60
1	A	71	MET	CG-SD-CE	7.63	117.69	100.90
1	E	623	ASP	CA-C-O	-7.15	108.64	120.80
1	F	408	ASP	CA-CB-CG	6.92	119.52	112.60
1	I	348	GLU	N-CA-CB	6.89	120.47	110.47
1	G	263	GLU	CB-CG-CD	6.82	124.20	112.60
1	J	54	GLU	CB-CG-CD	6.80	124.16	112.60
1	I	348	GLU	CG-CD-OE2	6.71	133.83	118.40
1	F	612	ARG	CA-CB-CG	6.64	127.39	114.10
1	I	350	SER	N-CA-CB	6.64	121.71	110.49
1	D	39	ARG	CG-CD-NE	6.63	126.60	112.00
1	B	412	GLU	CB-CA-C	-6.54	103.11	111.22
1	L	216	GLU	CG-CD-OE1	6.52	133.39	118.40
1	I	361	ASP	CA-CB-CG	6.47	119.07	112.60
1	F	559	ARG	N-CA-CB	6.45	121.47	110.50
1	C	100	MET	CG-SD-CE	6.44	115.08	100.90
1	E	92	ARG	CB-CG-CD	6.43	126.09	111.30
1	H	302	LYS	CA-CB-CG	6.42	126.93	114.10
1	J	509	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	680	ARG	N-CA-CB	-6.38	100.97	110.61
1	B	557	THR	CA-CB-OG1	6.37	119.15	109.60
1	A	474	PHE	CA-CB-CG	6.31	120.11	113.80
1	F	582	GLY	CA-C-O	-6.21	114.80	121.88
1	C	103	ILE	CA-CB-CG1	6.04	120.66	110.40
1	A	540	ARG	CA-CB-CG	-6.01	102.08	114.10
1	C	101	ARG	CG-CD-NE	-5.95	98.90	112.00
1	D	101	ARG	CB-CA-C	-5.78	98.92	110.42
1	A	35	THR	CA-CB-OG1	-5.77	100.95	109.60
1	C	31	ASP	CA-CB-CG	5.76	118.36	112.60
1	D	510	GLU	CB-CG-CD	-5.74	102.84	112.60
1	A	680	ARG	CB-CA-C	5.73	119.86	110.17
1	C	254	ARG	CG-CD-NE	5.73	124.60	112.00
1	C	259	ASN	CA-CB-CG	5.70	118.30	112.60
1	E	251	ARG	CA-CB-CG	5.70	125.50	114.10
1	E	56	ARG	CB-CG-CD	5.65	124.29	111.30
1	C	254	ARG	CA-CB-CG	5.54	125.19	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	651	THR	CA-CB-CG2	5.47	119.80	110.50
1	A	28	ASP	CA-CB-CG	5.46	118.06	112.60
1	I	348	GLU	CG-CD-OE1	-5.45	105.86	118.40
1	C	507	LYS	CG-CD-CE	5.45	123.83	111.30
1	C	259	ASN	CB-CA-C	5.44	119.52	110.81
1	F	68	ARG	CB-CG-CD	5.44	123.82	111.30
1	D	642	GLY	CA-C-N	5.44	135.06	121.80
1	D	642	GLY	C-N-CA	5.44	135.06	121.80
1	L	655	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	D	558	PHE	N-CA-C	-5.40	107.70	114.56
1	D	628	CYS	CB-CA-C	-5.39	109.89	117.23
1	I	137	LYS	CA-CB-CG	5.37	124.84	114.10
1	C	507	LYS	CB-CG-CD	5.35	123.60	111.30
1	C	314	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	K	408	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	274	ASP	CA-CB-CG	5.30	117.90	112.60
1	I	225	LYS	CB-CG-CD	5.30	123.48	111.30
1	C	79	PHE	CA-C-N	5.28	131.62	121.54
1	C	79	PHE	C-N-CA	5.28	131.62	121.54
1	L	95	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	60	ARG	CG-CD-NE	-5.27	100.41	112.00
1	F	135	ASP	CB-CA-C	5.25	119.25	110.44
1	K	254	ARG	CA-CB-CG	5.24	124.59	114.10
1	K	620	THR	OG1-CB-CG2	5.23	119.77	109.30
1	D	274	ASP	CA-CB-CG	5.22	117.82	112.60
1	J	513	GLN	CB-CA-C	5.21	116.88	108.91
1	E	48	ARG	CA-CB-CG	5.20	124.50	114.10
1	B	636	PRO	N-CA-CB	-5.20	97.79	103.25
1	A	177	VAL	N-CA-CB	5.20	116.19	110.53
1	L	361	ASP	CA-CB-CG	5.19	117.79	112.60
1	L	581	CYS	CB-CA-C	5.19	120.75	110.42
1	A	60	ARG	CA-CB-CG	5.18	124.47	114.10
1	B	101	ARG	CG-CD-NE	5.17	123.38	112.00
1	J	88	LYS	CA-CB-CG	5.15	124.41	114.10
1	F	558	PHE	CA-C-N	5.13	130.93	121.70
1	F	558	PHE	C-N-CA	5.13	130.93	121.70
1	F	127	SER	N-CA-C	-5.10	99.94	110.80
1	F	617	LEU	CB-CG-CD2	5.09	125.97	110.70
1	C	274	ASP	CA-CB-CG	5.08	117.68	112.60
1	I	632	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	215	PHE	N-CA-CB	-5.03	103.26	110.65
1	L	257	ARG	NE-CZ-NH2	5.02	123.72	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	274	ASP	CA-CB-CG	5.02	117.62	112.60
1	H	95	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ARG	Sidechain
1	B	56	ARG	Sidechain
1	D	34	LEU	Mainchain
1	D	473	ARG	Sidechain
1	D	631	ARG	Sidechain
1	E	221	ALA	Peptide
1	E	556	ARG	Sidechain
1	E	631	ARG	Sidechain
1	F	127	SER	Mainchain
1	F	221	ALA	Peptide
1	F	558	PHE	Peptide
1	F	92	ARG	Sidechain
1	G	221	ALA	Peptide
1	H	221	ALA	Peptide
1	H	257	ARG	Sidechain
1	J	221	ALA	Peptide
1	J	460	ARG	Sidechain
1	K	221	ALA	Peptide
1	L	221	ALA	Peptide
1	L	251	ARG	Sidechain

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	5377	0	5284	136	3
1	B	5330	0	5242	111	0
1	C	5358	0	5270	133	3
1	D	5373	0	5281	120	1
1	E	5450	0	5348	142	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	5421	0	5324	152	0
1	G	5431	0	5334	98	1
1	H	5450	0	5348	99	1
1	I	5442	0	5341	108	0
1	J	5431	0	5334	113	1
1	K	5442	0	5342	106	1
1	L	5431	0	5333	119	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	12	0	18	0	0
3	D	8	0	12	0	0
3	F	4	0	6	0	0
3	H	4	0	6	0	0
4	A	31	0	0	0	0
4	B	25	0	0	0	0
4	C	23	0	0	1	0
4	D	13	0	0	0	0
4	E	14	0	0	2	0
4	F	12	0	0	1	0
4	G	8	0	0	0	0
4	H	6	0	0	0	0
4	I	8	0	0	1	0
4	J	6	0	0	1	0
4	K	1	0	0	0	0
4	L	18	0	0	1	0
All	All	65153	0	63823	1343	6

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 10.

All (1343) 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:J:208:HIS:HB3	1:J:581:CYS:SG	1.38	1.60
1:A:132:HIS:CG	1:A:222:ILE:HD11	1.41	1.50
1:J:581:CYS:SG	1:J:622:ASN:HB3	1.55	1.46
1:B:28:ASP:OD1	1:B:56:ARG:NH1	1.60	1.33
1:B:493:ASP:O	1:D:101:ARG:HG2	1.34	1.27
1:B:101:ARG:HD2	1:D:493:ASP:O	1.36	1.26
1:H:349:SER:OG	1:H:361:ASP:OD1	1.54	1.25
1:F:349:SER:OG	1:F:361:ASP:OD1	1.53	1.24
1:A:132:HIS:CG	1:A:222:ILE:CD1	2.20	1.23
1:F:126:LEU:O	1:F:127:SER:O	1.57	1.23
1:I:208:HIS:CB	1:I:581:CYS:SG	2.27	1.23
1:B:319:VAL:CG1	1:B:412:GLU:O	1.87	1.23
1:J:208:HIS:CB	1:J:581:CYS:SG	2.26	1.22
1:F:100:MET:O	1:F:133:ARG:NH2	1.72	1.21
1:I:100:MET:O	1:I:133:ARG:NH2	1.75	1.19
1:B:28:ASP:CG	1:B:56:ARG:NH1	1.86	1.18
1:D:124:TYR:O	1:D:128:VAL:HG23	1.40	1.17
1:B:101:ARG:HB3	1:D:494:ALA:HA	1.24	1.15
1:A:678:VAL:HG12	1:A:679:PRO:HD2	1.26	1.15
1:C:549:THR:O	1:C:627:TYR:CE2	2.01	1.14
1:E:579:CYS:SG	1:E:635:TYR:HE2	1.71	1.13
1:J:161:ILE:HG21	1:J:462:MET:HE2	1.23	1.13
1:E:17:PRO:HD2	1:E:20:MET:HE3	1.25	1.12
1:J:581:CYS:SG	1:J:622:ASN:CB	2.36	1.12
1:I:208:HIS:HB2	1:I:581:CYS:SG	1.90	1.10
1:J:12:ASP:OD2	1:J:460:ARG:NH1	1.83	1.10
1:A:132:HIS:ND1	1:A:222:ILE:HD11	1.67	1.09
1:I:415:ILE:HG22	1:I:648:LEU:HD21	1.35	1.09
1:B:493:ASP:O	1:D:101:ARG:CG	2.00	1.08
1:A:366:GLY:O	1:A:370:LEU:HD13	1.52	1.08
1:K:620:THR:OG1	1:K:629:GLY:C	1.98	1.07
1:D:39:ARG:HB3	1:D:40:PRO:HD3	1.19	1.06
1:A:678:VAL:HG12	1:A:679:PRO:CD	1.83	1.06
1:I:209:TRP:N	1:I:581:CYS:SG	2.30	1.05
1:A:366:GLY:O	1:A:370:LEU:CD1	2.06	1.04
1:E:250:ASN:O	1:E:251:ARG:HD3	1.58	1.03
1:E:146:GLU:HB3	1:E:460:ARG:HD2	1.40	1.03
1:H:579:CYS:SG	1:H:630:VAL:HG21	1.97	1.03
1:B:319:VAL:HG11	1:B:412:GLU:O	1.58	1.02
1:D:38:TYR:HE2	1:G:167:VAL:HG11	1.23	1.02
1:C:615:GLN:NE2	1:C:634:LEU:HB2	1.73	1.02
1:E:552:ILE:CG2	1:E:582:GLY:HA3	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:LEU:HD12	4:E:803:HOH:O	1.59	1.00
1:C:3:TYR:HB3	1:C:103:ILE:HD11	1.44	0.99
1:A:272:LYS:HE3	1:I:382:GLU:OE2	1.62	0.99
1:J:161:ILE:HG21	1:J:462:MET:CE	1.91	0.98
1:B:615:GLN:NE2	1:B:633:ARG:HB2	1.78	0.98
1:F:60:ARG:NE	1:F:104:GLU:OE2	1.96	0.98
1:L:253:GLN:HG2	1:L:510:GLU:OE2	1.64	0.97
1:D:38:TYR:CE2	1:G:167:VAL:HG11	1.98	0.97
1:A:132:HIS:CB	1:A:222:ILE:CD1	2.43	0.97
1:I:208:HIS:HB3	1:I:581:CYS:SG	2.04	0.96
1:A:67:LEU:CD1	1:A:96:ILE:HD13	1.96	0.95
1:L:101:ARG:CZ	1:L:105:GLU:OE2	2.15	0.94
1:F:556:ARG:NE	1:F:623:ASP:OD2	1.99	0.94
1:H:257:ARG:NH2	1:I:304:ASP:OD1	2.00	0.94
1:E:20:MET:HE2	1:J:167:VAL:HG22	1.46	0.94
1:F:60:ARG:CZ	1:F:104:GLU:OE2	2.16	0.93
1:I:208:HIS:C	1:I:581:CYS:SG	2.51	0.93
1:I:579:CYS:SG	1:I:630:VAL:HG21	2.09	0.93
1:K:620:THR:CG2	1:K:629:GLY:HA3	1.98	0.92
1:C:549:THR:O	1:C:627:TYR:HE2	1.43	0.92
1:F:622:ASN:OD1	1:F:629:GLY:HA3	1.69	0.92
1:K:620:THR:HG23	1:K:629:GLY:HA3	1.52	0.92
1:I:345:ASN:O	1:I:349:SER:O	1.87	0.92
1:D:39:ARG:HB3	1:D:40:PRO:CD	2.01	0.91
1:G:349:SER:OG	1:G:356:ARG:NH1	2.02	0.91
1:H:579:CYS:SG	1:H:630:VAL:CG2	2.59	0.90
1:I:579:CYS:SG	1:I:630:VAL:CG2	2.60	0.90
1:J:515:MET:HE1	1:J:523:PHE:CD2	2.07	0.89
1:C:349:SER:HB3	1:C:356:ARG:HH11	1.35	0.88
1:C:549:THR:O	1:C:627:TYR:CD2	2.27	0.88
1:C:615:GLN:HE21	1:C:634:LEU:HB2	1.33	0.88
1:C:615:GLN:HE21	1:C:634:LEU:CB	1.86	0.87
1:J:581:CYS:HG	1:J:622:ASN:HB3	0.93	0.86
1:F:131:LEU:HD21	1:F:141:LEU:HD21	1.57	0.86
1:F:70:PRO:HD3	1:F:92:ARG:HG2	1.58	0.85
1:J:25:SER:HB3	1:J:57:ILE:HD11	1.59	0.85
1:L:192:ARG:CZ	1:L:251:ARG:NH1	2.39	0.85
1:C:349:SER:OG	1:C:360:GLY:O	1.94	0.85
1:D:217:ALA:HA	1:D:351:ILE:HG21	1.59	0.85
1:B:28:ASP:HB2	1:B:56:ARG:CZ	2.06	0.84
1:D:124:TYR:O	1:D:128:VAL:CG2	2.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ASP:OD1	1:D:556:ARG:NH2	2.11	0.84
1:J:454:SER:OG	1:J:680:ARG:HD3	1.78	0.83
1:L:192:ARG:NH2	1:L:251:ARG:HH11	1.76	0.83
1:F:60:ARG:NH1	1:F:104:GLU:CD	2.37	0.83
1:E:552:ILE:HG21	1:E:582:GLY:HA3	1.61	0.82
1:D:628:CYS:SG	1:D:629:GLY:N	2.52	0.82
1:F:556:ARG:CG	1:F:623:ASP:OD2	2.28	0.82
1:L:579:CYS:SG	1:L:627:TYR:OH	2.35	0.82
1:A:132:HIS:CD2	1:A:222:ILE:HD11	2.12	0.81
1:C:3:TYR:CB	1:C:103:ILE:HD11	2.10	0.81
1:F:60:ARG:NH1	1:F:104:GLU:OE1	2.12	0.81
1:C:348:GLU:HB2	1:C:363:HIS:HB3	1.62	0.81
1:I:621:CYS:C	1:I:631:ARG:NH1	2.38	0.81
1:L:72:SER:OG	1:L:89:ILE:CD1	2.29	0.81
1:L:540:ARG:O	1:L:540:ARG:HG3	1.81	0.81
1:A:349:SER:OG	1:A:360:GLY:O	1.99	0.81
1:F:60:ARG:HH11	1:F:104:GLU:CD	1.89	0.80
1:F:552:ILE:HD12	1:F:582:GLY:C	2.06	0.80
1:H:581:CYS:SG	1:H:622:ASN:OD1	2.40	0.80
1:J:231:LEU:HD11	1:J:579:CYS:CB	2.11	0.80
1:A:333:PHE:CD1	1:F:333:PHE:CE1	2.68	0.80
1:G:454:SER:OG	1:G:680:ARG:HD2	1.82	0.80
1:B:615:GLN:HE22	1:B:633:ARG:HB2	1.46	0.80
1:L:349:SER:OG	1:L:360:GLY:O	2.00	0.80
1:C:215:PHE:CD1	1:C:216:GLU:HG3	2.16	0.80
1:C:348:GLU:HA	1:C:363:HIS:HB3	1.62	0.80
1:D:100:MET:SD	1:D:101:ARG:NH2	2.54	0.80
1:B:28:ASP:CB	1:B:56:ARG:CZ	2.40	0.79
1:B:349:SER:OG	1:B:360:GLY:O	2.00	0.79
1:E:349:SER:HB3	1:E:361:ASP:HA	1.64	0.79
1:F:267:GLU:HG3	4:F:805:HOH:O	1.82	0.79
1:J:349:SER:OG	1:J:360:GLY:O	2.01	0.79
1:L:81:LEU:HD12	1:L:81:LEU:H	1.47	0.79
1:D:251:ARG:HE	1:L:251:ARG:HD2	1.47	0.79
1:D:349:SER:OG	1:D:360:GLY:O	1.98	0.79
1:I:117:ILE:HD11	1:I:122:PHE:HB2	1.65	0.78
1:K:349:SER:OG	1:K:360:GLY:O	2.01	0.78
1:F:60:ARG:NH1	1:F:104:GLU:OE2	2.17	0.78
1:J:161:ILE:CG2	1:J:462:MET:HE2	2.10	0.78
1:J:267:GLU:O	1:J:285:ARG:NH2	2.14	0.78
1:F:132:HIS:ND1	1:F:222:ILE:HD13	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLU:HB2	1:B:351:ILE:HG23	1.66	0.78
1:C:215:PHE:HD1	1:C:216:GLU:HG3	1.48	0.78
1:A:321:GLN:O	1:A:321:GLN:NE2	2.16	0.78
1:E:579:CYS:SG	1:E:635:TYR:CE2	2.59	0.77
1:F:232:PHE:CD1	1:F:348:GLU:OE1	2.37	0.77
1:I:208:HIS:CA	1:I:581:CYS:SG	2.72	0.77
1:A:67:LEU:HD11	1:A:96:ILE:HD13	1.66	0.77
1:D:164:GLU:OE2	1:G:37:ARG:NH1	2.18	0.77
1:H:257:ARG:HH22	1:I:304:ASP:CG	1.92	0.77
1:K:618:VAL:HG23	1:K:632:ASP:OD1	1.84	0.77
1:F:349:SER:HB3	1:F:361:ASP:HA	1.67	0.77
1:J:231:LEU:HD11	1:J:579:CYS:HB3	1.67	0.77
1:F:556:ARG:CD	1:F:623:ASP:OD2	2.31	0.77
1:K:620:THR:HG23	1:K:628:CYS:O	1.85	0.77
1:J:161:ILE:CG2	1:J:462:MET:CE	2.63	0.76
1:K:620:THR:CG2	1:K:629:GLY:CA	2.63	0.76
1:A:132:HIS:HB3	1:A:222:ILE:HD12	1.67	0.76
1:B:319:VAL:HG12	1:B:412:GLU:O	1.85	0.76
1:H:349:SER:HB3	1:H:361:ASP:HA	1.66	0.76
1:L:216:GLU:OE2	1:L:356:ARG:NH2	2.16	0.76
1:I:579:CYS:SG	1:I:579:CYS:O	2.42	0.76
1:E:67:LEU:HB3	1:E:71:MET:HE2	1.68	0.76
1:K:618:VAL:CG2	1:K:632:ASP:OD1	2.34	0.76
1:E:43:PRO:O	1:E:47:ASN:ND2	2.19	0.76
1:A:333:PHE:CE1	1:F:333:PHE:CE1	2.74	0.76
1:D:251:ARG:NE	1:L:251:ARG:HD2	2.01	0.76
1:K:238:GLN:HB3	1:K:578:PHE:CZ	2.20	0.75
1:L:68:ARG:HD2	1:L:68:ARG:C	2.10	0.75
1:G:231:LEU:HD11	1:G:580:GLY:HA3	1.69	0.74
1:C:615:GLN:NE2	1:C:634:LEU:CB	2.46	0.74
1:E:20:MET:HE2	1:J:167:VAL:CG2	2.18	0.74
1:A:28:ASP:OD1	1:A:56:ARG:NH2	2.21	0.74
1:D:94:ILE:HD13	1:D:128:VAL:HG11	1.69	0.74
1:D:349:SER:HB2	1:D:361:ASP:HA	1.70	0.73
1:E:208:HIS:HB3	1:E:581:CYS:HB2	1.70	0.73
1:L:72:SER:OG	1:L:89:ILE:HD13	1.87	0.73
1:C:220:ARG:O	1:C:220:ARG:HG2	1.88	0.73
1:D:37:ARG:NH1	1:G:164:GLU:OE2	2.19	0.73
1:K:620:THR:OG1	1:K:629:GLY:CA	2.36	0.73
1:C:330:ASN:ND2	1:F:332:ILE:HD13	2.02	0.73
1:I:621:CYS:O	1:I:631:ARG:NH1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:VAL:HG22	1:D:213:TYR:CD1	2.23	0.73
1:F:126:LEU:C	1:F:127:SER:O	2.30	0.73
1:F:132:HIS:CD2	1:F:222:ILE:HG12	2.24	0.73
1:F:131:LEU:HD21	1:F:141:LEU:CD2	2.19	0.72
1:I:415:ILE:HG22	1:I:648:LEU:CD2	2.16	0.72
1:I:621:CYS:C	1:I:631:ARG:HH12	1.95	0.72
1:C:82:PHE:O	1:C:87:ARG:NH2	2.23	0.72
1:K:620:THR:CB	1:K:629:GLY:HA3	2.18	0.72
1:A:132:HIS:HB3	1:A:222:ILE:CD1	2.17	0.72
1:F:132:HIS:ND1	1:F:222:ILE:CD1	2.53	0.72
1:C:217:ALA:HB3	1:C:223:VAL:HG23	1.71	0.72
1:F:552:ILE:HD13	1:F:552:ILE:H	1.55	0.72
1:D:39:ARG:CB	1:D:40:PRO:HD3	2.07	0.72
1:A:67:LEU:CD1	1:A:96:ILE:CD1	2.68	0.72
1:A:272:LYS:CE	1:I:382:GLU:OE2	2.37	0.72
1:A:161:ILE:HD13	1:A:462:MET:HE3	1.72	0.71
1:C:28:ASP:OD1	1:C:56:ARG:NH2	2.23	0.71
1:C:161:ILE:HD13	1:C:462:MET:HE3	1.72	0.71
1:A:450:TYR:CD1	1:A:678:VAL:CG2	2.74	0.71
1:F:161:ILE:HD13	1:F:462:MET:HE3	1.72	0.71
1:F:4:LYS:HE2	1:F:139:LEU:HD13	1.73	0.71
1:E:230:GLU:HG2	1:E:641:MET:HE3	1.71	0.71
1:F:98:MET:HE3	1:F:132:HIS:O	1.89	0.71
1:A:581:CYS:SG	1:A:581:CYS:O	2.49	0.71
1:C:310:ARG:O	1:C:314:ARG:HG3	1.89	0.71
1:I:161:ILE:HD13	1:I:462:MET:HE3	1.73	0.71
1:K:242:ARG:HD2	1:K:578:PHE:CZ	2.25	0.71
1:B:161:ILE:HD13	1:B:462:MET:HE3	1.72	0.70
1:C:349:SER:HB3	1:C:356:ARG:NH1	2.05	0.70
1:E:70:PRO:HD3	1:E:92:ARG:HD2	1.72	0.70
1:H:310:ARG:O	1:H:314:ARG:HG3	1.91	0.70
1:L:579:CYS:SG	1:L:630:VAL:HG21	2.30	0.70
1:A:254:ARG:CB	1:A:254:ARG:HH11	2.04	0.70
1:A:366:GLY:O	1:A:370:LEU:HD12	1.88	0.70
1:B:554:PHE:HD1	1:B:554:PHE:H	1.36	0.70
1:A:331:ARG:CZ	1:F:330:ASN:HB3	2.22	0.70
1:C:132:HIS:CG	1:C:222:ILE:HD11	2.26	0.70
1:E:579:CYS:HA	1:E:630:VAL:HG21	1.74	0.70
1:D:613:VAL:O	1:D:614:VAL:C	2.34	0.70
1:F:581:CYS:SG	1:F:623:ASP:C	2.75	0.70
1:H:257:ARG:NH2	1:I:304:ASP:CG	2.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:ILE:HD13	1:G:462:MET:HE3	1.72	0.69
1:L:192:ARG:CZ	1:L:251:ARG:HH11	2.04	0.69
1:H:161:ILE:HD13	1:H:462:MET:HE3	1.73	0.69
1:C:348:GLU:CB	1:C:363:HIS:HB3	2.21	0.69
1:A:310:ARG:O	1:A:314:ARG:HG3	1.91	0.69
1:E:620:THR:N	1:E:628:CYS:HB3	2.08	0.69
1:C:347:ILE:O	1:C:348:GLU:HB3	1.93	0.68
1:C:348:GLU:CA	1:C:363:HIS:HB3	2.23	0.68
1:D:60:ARG:NH1	1:D:104:GLU:OE1	2.26	0.68
1:K:161:ILE:HD13	1:K:462:MET:HE3	1.74	0.68
1:C:132:HIS:CG	1:C:222:ILE:CD1	2.75	0.68
1:G:37:ARG:HD2	1:G:37:ARG:C	2.18	0.68
1:L:161:ILE:HD13	1:L:462:MET:HE3	1.75	0.68
1:C:3:TYR:HB3	1:C:103:ILE:CD1	2.21	0.68
1:G:37:ARG:C	1:G:37:ARG:CD	2.67	0.68
1:E:24:LYS:HD3	1:E:54:GLU:OE2	1.92	0.68
1:E:578:PHE:HB3	1:E:579:CYS:SG	2.34	0.68
1:F:37:ARG:CD	1:F:37:ARG:C	2.67	0.68
1:L:132:HIS:ND1	1:L:222:ILE:HD13	2.09	0.68
1:D:231:LEU:HD11	1:D:629:GLY:HA2	1.73	0.68
1:F:132:HIS:CG	1:F:222:ILE:HG12	2.29	0.67
1:K:242:ARG:CD	1:K:578:PHE:CZ	2.77	0.67
1:K:620:THR:OG1	1:K:629:GLY:HA3	1.94	0.67
1:E:146:GLU:HB3	1:E:460:ARG:CD	2.21	0.67
1:E:487:GLN:OE1	1:E:540:ARG:NH1	2.28	0.67
1:A:450:TYR:CD1	1:A:678:VAL:HG23	2.29	0.67
1:B:555:GLU:O	1:B:558:PHE:HD2	1.77	0.67
1:A:678:VAL:CG1	1:A:679:PRO:CD	2.68	0.67
1:A:46:GLN:OE1	1:A:46:GLN:O	2.12	0.66
1:B:554:PHE:CD1	1:B:554:PHE:N	2.64	0.66
1:C:280:ARG:HH21	1:H:154:ASP:CG	2.03	0.66
1:I:97:PHE:O	1:I:133:ARG:NH1	2.27	0.66
1:A:221:ALA:O	1:A:222:ILE:HG22	1.96	0.66
1:B:552:ILE:HG23	1:B:582:GLY:HA3	1.77	0.66
1:G:629:GLY:O	1:G:630:VAL:HG22	1.96	0.66
1:L:192:ARG:NH2	1:L:251:ARG:NH1	2.44	0.66
1:L:68:ARG:HD2	1:L:68:ARG:O	1.94	0.66
1:D:164:GLU:CD	1:G:37:ARG:HH11	2.04	0.66
1:F:37:ARG:C	1:F:37:ARG:HD2	2.21	0.66
1:F:98:MET:HE1	1:F:132:HIS:CB	2.26	0.66
1:L:629:GLY:O	1:L:630:VAL:HG22	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:349:SER:HB3	1:G:361:ASP:OD1	1.95	0.66
1:C:137:LYS:HD3	1:C:137:LYS:C	2.21	0.65
1:E:552:ILE:HG23	1:E:582:GLY:HA3	1.77	0.65
1:F:104:GLU:OE1	1:F:105:GLU:HG3	1.96	0.65
1:F:629:GLY:O	1:F:630:VAL:HG22	1.96	0.65
1:H:577:ASN:N	1:H:627:TYR:HH	1.94	0.65
1:H:629:GLY:O	1:H:630:VAL:HG22	1.97	0.65
1:K:629:GLY:O	1:K:630:VAL:HG22	1.97	0.65
1:E:581:CYS:HA	1:E:622:ASN:HB2	1.78	0.65
1:J:268:GLY:HA2	1:J:285:ARG:NH1	2.11	0.65
1:E:621:CYS:HG	1:E:628:CYS:HG	1.42	0.65
1:D:37:ARG:HD3	1:D:37:ARG:C	2.22	0.65
1:D:168:VAL:HG21	1:G:37:ARG:NH1	2.11	0.65
1:F:93:LEU:HD13	1:F:125:ALA:CB	2.26	0.65
1:C:349:SER:HB2	1:C:361:ASP:OD1	1.97	0.65
1:J:629:GLY:O	1:J:630:VAL:HG22	1.96	0.64
1:F:556:ARG:HG2	1:F:623:ASP:OD2	1.96	0.64
1:G:680:ARG:HG2	1:G:680:ARG:HH21	1.60	0.64
1:L:101:ARG:NH2	1:L:105:GLU:OE2	2.29	0.64
1:L:232:PHE:CE1	1:L:348:GLU:OE2	2.50	0.64
1:B:219:ASN:HD21	1:D:609:GLU:HG2	1.63	0.64
1:J:25:SER:HB3	1:J:57:ILE:CD1	2.27	0.64
1:H:132:HIS:ND1	1:H:222:ILE:HD13	2.13	0.64
1:G:304:ASP:CG	1:L:257:ARG:HH12	2.06	0.64
1:F:132:HIS:CG	1:F:222:ILE:CD1	2.81	0.63
1:I:349:SER:OG	1:I:356:ARG:HD2	1.99	0.63
1:F:37:ARG:CD	1:F:37:ARG:O	2.45	0.63
1:F:37:ARG:O	1:F:37:ARG:HD3	1.97	0.63
1:L:579:CYS:HG	1:L:627:TYR:HH	1.45	0.63
1:E:349:SER:CB	1:E:361:ASP:HA	2.28	0.63
1:D:349:SER:CB	1:D:361:ASP:HA	2.27	0.63
1:E:250:ASN:C	1:E:251:ARG:HD3	2.22	0.63
1:K:550:VAL:HG13	1:K:578:PHE:HB2	1.80	0.63
1:K:132:HIS:ND1	1:K:222:ILE:HD13	2.13	0.63
1:E:132:HIS:ND1	1:E:222:ILE:HD13	2.14	0.63
1:I:579:CYS:SG	1:I:630:VAL:HG23	2.38	0.63
1:I:629:GLY:O	1:I:630:VAL:HG22	1.99	0.63
1:A:37:ARG:HD2	1:A:37:ARG:O	1.99	0.62
1:A:46:GLN:OE1	1:A:46:GLN:C	2.42	0.62
1:A:62:ILE:HD13	1:A:63:ALA:H	1.64	0.62
1:A:450:TYR:CD1	1:A:678:VAL:HG21	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:TYR:OH	1:C:141:LEU:HD21	1.99	0.62
1:G:37:ARG:CD	1:G:37:ARG:O	2.47	0.62
1:A:615:GLN:O	1:E:220:ARG:NH2	2.28	0.62
1:A:678:VAL:HG12	1:A:679:PRO:HD3	1.75	0.62
1:D:19:PHE:HZ	1:D:38:TYR:CD2	2.18	0.62
1:F:62:ILE:HD12	1:F:105:GLU:HG2	1.80	0.62
1:J:349:SER:CB	1:J:361:ASP:HA	2.30	0.62
1:L:400:TYR:O	1:L:404:SER:HB2	2.00	0.62
1:B:146:GLU:OE2	1:B:558:PHE:HE1	1.83	0.62
1:G:132:HIS:ND1	1:G:222:ILE:HD13	2.14	0.62
1:J:132:HIS:ND1	1:J:222:ILE:HD13	2.13	0.62
1:C:400:TYR:O	1:C:404:SER:HB2	2.00	0.62
1:E:208:HIS:CB	1:E:581:CYS:HB2	2.30	0.62
1:J:179:PRO:HB3	4:J:805:HOH:O	1.97	0.62
1:L:349:SER:CB	1:L:361:ASP:HA	2.30	0.62
1:B:400:TYR:O	1:B:404:SER:HB2	2.00	0.62
1:C:216:GLU:OE2	1:C:356:ARG:NH2	2.26	0.62
1:G:349:SER:HB2	1:G:361:ASP:HA	1.81	0.62
1:K:349:SER:HB3	1:K:356:ARG:HH11	1.63	0.62
1:L:232:PHE:CD1	1:L:348:GLU:OE2	2.53	0.62
1:B:493:ASP:O	1:D:101:ARG:HG3	1.96	0.62
1:D:15:ARG:NH1	1:G:159:GLU:OE2	2.33	0.62
1:D:613:VAL:O	1:D:614:VAL:O	2.16	0.62
1:F:98:MET:CE	1:F:132:HIS:O	2.48	0.62
1:G:400:TYR:O	1:G:404:SER:HB2	2.00	0.62
1:C:77:GLU:OE1	1:H:156:ARG:NH2	2.32	0.61
1:F:349:SER:CB	1:F:361:ASP:HA	2.30	0.61
1:K:400:TYR:O	1:K:404:SER:HB2	2.00	0.61
1:K:579:CYS:HA	1:K:627:TYR:CE2	2.35	0.61
1:B:349:SER:HB3	1:B:356:ARG:HH11	1.65	0.61
1:D:557:THR:HG22	1:D:557:THR:O	2.01	0.61
1:F:400:TYR:O	1:F:404:SER:HB2	2.00	0.61
1:H:400:TYR:O	1:H:404:SER:HB2	2.00	0.61
1:A:3:TYR:HB3	1:A:103:ILE:CG2	2.30	0.61
1:A:631:ARG:O	1:A:632:ASP:HB2	1.99	0.61
1:B:219:ASN:ND2	1:D:609:GLU:HG2	2.16	0.61
1:I:639:LYS:HE3	1:I:643:PHE:CZ	2.36	0.61
1:J:400:TYR:O	1:J:404:SER:HB2	2.00	0.61
1:A:254:ARG:HH11	1:A:254:ARG:HB3	1.65	0.61
1:J:349:SER:HB3	1:J:356:ARG:HH11	1.65	0.61
1:D:400:TYR:O	1:D:404:SER:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:ILE:HD11	1:F:403:HIS:HB3	1.83	0.61
1:I:117:ILE:HD11	1:I:122:PHE:CB	2.30	0.61
1:C:94:ILE:HD13	1:C:128:VAL:HB	1.81	0.61
1:J:349:SER:HB2	1:J:361:ASP:HA	1.82	0.61
1:A:400:TYR:O	1:A:404:SER:HB2	2.00	0.61
1:C:11:TYR:OH	1:C:141:LEU:CD2	2.49	0.61
1:D:227:ARG:NH2	1:D:637:ASP:O	2.34	0.61
1:I:227:ARG:NH2	1:I:637:ASP:O	2.34	0.61
1:C:227:ARG:NH2	1:C:637:ASP:O	2.34	0.61
1:H:349:SER:CB	1:H:361:ASP:HA	2.31	0.61
1:I:400:TYR:O	1:I:404:SER:HB2	2.00	0.61
1:H:208:HIS:CB	1:H:581:CYS:HB2	2.31	0.61
1:J:208:HIS:CG	1:J:581:CYS:SG	2.93	0.61
1:C:103:ILE:HG22	1:C:135:ASP:OD2	2.00	0.61
1:E:240:ILE:HD11	1:E:403:HIS:HB3	1.83	0.61
1:E:661:THR:CG2	1:E:664:MET:HE3	2.31	0.61
1:F:65:PRO:HB2	1:F:96:ILE:CD1	2.30	0.61
1:I:240:ILE:HD11	1:I:403:HIS:HB3	1.82	0.61
1:A:240:ILE:HD11	1:A:403:HIS:HB3	1.83	0.60
1:E:158:PHE:CD1	1:E:462:MET:HE1	2.36	0.60
1:L:240:ILE:HD11	1:L:403:HIS:HB3	1.83	0.60
1:A:227:ARG:NH2	1:A:637:ASP:O	2.34	0.60
1:A:349:SER:HB2	1:A:361:ASP:HA	1.83	0.60
1:B:240:ILE:HD11	1:B:403:HIS:HB3	1.83	0.60
1:B:349:SER:CB	1:B:361:ASP:HA	2.30	0.60
1:E:400:TYR:O	1:E:404:SER:HB2	2.01	0.60
1:G:227:ARG:NH2	1:G:637:ASP:O	2.34	0.60
1:H:227:ARG:NH2	1:H:637:ASP:O	2.34	0.60
1:J:227:ARG:NH2	1:J:637:ASP:O	2.34	0.60
1:K:227:ARG:NH2	1:K:637:ASP:O	2.34	0.60
1:L:192:ARG:NH1	1:L:251:ARG:HE	1.99	0.60
1:L:227:ARG:NH2	1:L:637:ASP:O	2.35	0.60
1:E:227:ARG:NH2	1:E:637:ASP:O	2.34	0.60
1:G:304:ASP:OD2	1:L:257:ARG:NH1	2.34	0.60
1:J:240:ILE:HD11	1:J:403:HIS:HB3	1.83	0.60
1:L:349:SER:HB2	1:L:361:ASP:HA	1.83	0.60
1:A:30:PRO:HD3	1:A:59:VAL:HG13	1.81	0.60
1:A:349:SER:CB	1:A:361:ASP:HA	2.31	0.60
1:D:240:ILE:HD11	1:D:403:HIS:HB3	1.83	0.60
1:K:349:SER:CB	1:K:361:ASP:HA	2.32	0.60
1:A:452:GLN:OE1	1:A:478:GLN:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:TYR:CZ	1:C:141:LEU:HD23	2.37	0.60
1:G:349:SER:CB	1:G:361:ASP:HA	2.31	0.60
1:H:240:ILE:HD11	1:H:403:HIS:HB3	1.83	0.60
1:B:227:ARG:NH2	1:B:637:ASP:O	2.34	0.60
1:A:307:ASP:OD1	1:A:310:ARG:NH1	2.29	0.59
1:B:349:SER:HB2	1:B:361:ASP:HA	1.83	0.59
1:C:330:ASN:ND2	1:F:332:ILE:CD1	2.65	0.59
1:G:37:ARG:O	1:G:37:ARG:HD3	2.02	0.59
1:H:208:HIS:HB3	1:H:581:CYS:HB2	1.84	0.59
1:K:349:SER:HB2	1:K:361:ASP:HA	1.83	0.59
1:I:117:ILE:HD11	1:I:122:PHE:CA	2.33	0.59
1:K:240:ILE:HD11	1:K:403:HIS:HB3	1.83	0.59
1:A:226:ASP:CG	1:A:634:LEU:CD1	2.75	0.59
1:F:227:ARG:NH2	1:F:637:ASP:O	2.35	0.59
1:F:552:ILE:HG23	1:F:582:GLY:HA3	1.84	0.59
1:A:81:LEU:O	1:A:87:ARG:HD2	2.03	0.59
1:C:348:GLU:HB2	1:C:363:HIS:CB	2.30	0.59
1:C:348:GLU:HG3	1:C:363:HIS:HD1	1.66	0.59
1:L:349:SER:HB3	1:L:356:ARG:HH11	1.67	0.59
1:C:132:HIS:CE1	1:C:222:ILE:HD11	2.37	0.59
1:G:240:ILE:HD11	1:G:403:HIS:HB3	1.83	0.59
1:C:330:ASN:HD21	1:F:332:ILE:HD13	1.66	0.59
1:C:349:SER:HG	1:C:361:ASP:HA	1.66	0.59
1:L:132:HIS:CG	1:L:222:ILE:CD1	2.85	0.59
1:F:30:PRO:HD3	1:F:59:VAL:HG13	1.85	0.58
1:I:579:CYS:HA	1:I:627:TYR:CE2	2.38	0.58
1:A:349:SER:HB3	1:A:356:ARG:HH11	1.67	0.58
1:D:30:PRO:HD3	1:D:59:VAL:HG13	1.85	0.58
1:K:620:THR:HG23	1:K:629:GLY:CA	2.25	0.58
1:D:81:LEU:O	1:D:87:ARG:HD2	2.03	0.58
1:C:44:GLU:HG2	1:H:169:PRO:HG2	1.85	0.58
1:D:349:SER:O	1:D:356:ARG:NH1	2.37	0.58
1:F:455:ASP:OD1	1:F:473:ARG:HG3	2.02	0.58
1:B:333:PHE:CZ	1:D:331:ARG:HB2	2.38	0.58
1:D:348:GLU:HA	1:D:363:HIS:HB3	1.84	0.58
1:E:17:PRO:CD	1:E:20:MET:HE3	2.17	0.58
1:G:62:ILE:CG2	1:G:64:LEU:HD13	2.34	0.58
1:J:30:PRO:HD3	1:J:59:VAL:HG13	1.86	0.58
1:K:30:PRO:HD3	1:K:59:VAL:HG13	1.86	0.58
1:F:101:ARG:H	1:F:101:ARG:HD2	1.69	0.58
1:H:552:ILE:HG23	1:H:582:GLY:HA3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:30:PRO:HD3	1:L:59:VAL:HG13	1.86	0.58
1:C:240:ILE:HD11	1:C:403:HIS:HB3	1.85	0.58
1:E:81:LEU:O	1:E:87:ARG:HD2	2.04	0.58
1:E:581:CYS:SG	1:E:622:ASN:ND2	2.76	0.58
1:J:81:LEU:O	1:J:87:ARG:HD2	2.04	0.58
1:J:552:ILE:HG23	1:J:582:GLY:HA3	1.86	0.58
1:B:615:GLN:HE22	1:B:634:LEU:H	1.51	0.57
1:D:631:ARG:HG3	1:D:633:ARG:HG3	1.85	0.57
1:F:81:LEU:O	1:F:87:ARG:HD2	2.04	0.57
1:H:81:LEU:O	1:H:87:ARG:HD2	2.04	0.57
1:A:132:HIS:CD2	1:A:222:ILE:CD1	2.79	0.57
1:B:615:GLN:HE21	1:B:633:ARG:HB2	1.68	0.57
1:E:231:LEU:CA	1:E:641:MET:HE1	2.34	0.57
1:E:581:CYS:SG	1:E:622:ASN:CG	2.87	0.57
1:H:30:PRO:HD3	1:H:59:VAL:HG13	1.85	0.57
1:G:81:LEU:O	1:G:87:ARG:HD2	2.04	0.57
1:D:615:GLN:HE22	1:D:633:ARG:HB2	1.69	0.57
1:G:30:PRO:HD3	1:G:59:VAL:HG13	1.85	0.57
1:I:30:PRO:HD3	1:I:59:VAL:HG13	1.86	0.57
1:I:132:HIS:NE2	1:I:222:ILE:HG21	2.19	0.57
1:L:69:ILE:HB	1:L:70:PRO:HD3	1.86	0.57
1:A:254:ARG:HB3	1:A:254:ARG:NH1	2.19	0.57
1:B:91:ALA:HB1	1:B:217:ALA:O	2.04	0.57
1:E:231:LEU:HD21	1:E:579:CYS:HB2	1.87	0.57
1:E:304:ASP:CG	1:F:257:ARG:HH12	2.12	0.57
1:I:349:SER:HB2	1:I:361:ASP:HA	1.87	0.57
1:L:253:GLN:CG	1:L:510:GLU:OE2	2.47	0.57
1:B:30:PRO:HD3	1:B:59:VAL:HG13	1.86	0.57
1:C:216:GLU:CD	1:C:356:ARG:HH22	2.12	0.57
1:E:579:CYS:HB3	1:E:630:VAL:HG11	1.86	0.57
1:L:81:LEU:HD12	1:L:81:LEU:N	2.17	0.57
1:B:81:LEU:O	1:B:87:ARG:HD2	2.05	0.57
1:C:552:ILE:HG23	1:C:582:GLY:HA3	1.87	0.57
1:D:357:GLN:HG2	1:E:416:LYS:NZ	2.19	0.57
1:E:69:ILE:HB	1:E:70:PRO:HD3	1.85	0.57
1:F:100:MET:HA	1:F:100:MET:HE2	1.86	0.57
1:K:552:ILE:HG23	1:K:582:GLY:HA3	1.86	0.57
1:E:526:GLU:OE2	1:E:578:PHE:CE2	2.58	0.57
1:E:552:ILE:HD12	1:E:556:ARG:HG2	1.87	0.57
1:G:218:SER:OG	1:G:220:ARG:HG3	2.05	0.57
1:A:226:ASP:CG	1:A:634:LEU:HD13	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:PRO:HD2	4:C:817:HOH:O	2.05	0.57
1:E:556:ARG:NH2	1:E:621:CYS:SG	2.78	0.57
1:F:132:HIS:CE1	1:F:222:ILE:HD13	2.40	0.57
1:D:69:ILE:HB	1:D:70:PRO:HD3	1.86	0.56
1:F:617:LEU:HD13	1:F:617:LEU:N	2.21	0.56
1:B:492:SER:O	1:B:493:ASP:HB2	2.06	0.56
1:C:349:SER:CB	1:C:361:ASP:HA	2.36	0.56
1:F:126:LEU:O	1:F:127:SER:C	2.40	0.56
1:K:81:LEU:O	1:K:87:ARG:HD2	2.05	0.56
1:L:81:LEU:H	1:L:81:LEU:CD1	2.15	0.56
1:D:91:ALA:HB2	1:D:216:GLU:OE2	2.05	0.56
1:C:492:SER:O	1:C:493:ASP:HB2	2.06	0.56
1:C:507:LYS:HE2	1:C:668:SER:OG	2.06	0.56
1:F:62:ILE:CD1	1:F:105:GLU:HG2	2.35	0.56
1:I:348:GLU:HA	1:I:363:HIS:HB3	1.85	0.56
1:J:515:MET:HE1	1:J:523:PHE:CE2	2.40	0.56
1:L:552:ILE:HG23	1:L:582:GLY:HA3	1.87	0.56
1:B:4:LYS:HE2	1:B:139:LEU:HD13	1.86	0.56
1:C:612:ARG:NH2	1:F:101:ARG:HB3	2.21	0.56
1:E:552:ILE:HD11	1:E:556:ARG:HB3	1.87	0.56
1:I:81:LEU:O	1:I:87:ARG:HD2	2.05	0.56
1:J:492:SER:O	1:J:493:ASP:HB2	2.06	0.56
1:C:349:SER:OG	1:C:361:ASP:HA	2.05	0.56
1:K:620:THR:HB	1:K:631:ARG:H	1.70	0.56
1:E:146:GLU:CB	1:E:460:ARG:HD2	2.24	0.56
1:E:231:LEU:HA	1:E:641:MET:HE1	1.87	0.56
1:K:492:SER:O	1:K:493:ASP:HB2	2.06	0.56
1:K:620:THR:HG21	1:K:630:VAL:H	1.71	0.56
1:B:216:GLU:HB2	1:B:351:ILE:CG2	2.35	0.56
1:B:348:GLU:HA	1:B:363:HIS:HB3	1.88	0.56
1:E:30:PRO:HD3	1:E:59:VAL:HG13	1.87	0.56
1:E:132:HIS:CG	1:E:222:ILE:CD1	2.89	0.56
1:E:492:SER:O	1:E:493:ASP:HB2	2.06	0.56
1:F:310:ARG:NH1	1:F:310:ARG:HG3	2.20	0.56
1:A:103:ILE:HG13	1:A:135:ASP:OD2	2.05	0.55
1:C:132:HIS:ND1	1:C:222:ILE:HD11	2.21	0.55
1:H:492:SER:O	1:H:493:ASP:HB2	2.06	0.55
1:K:242:ARG:NE	1:K:578:PHE:CZ	2.75	0.55
1:K:579:CYS:HA	1:K:627:TYR:HE2	1.69	0.55
1:B:633:ARG:HH21	1:D:616:ASP:HB3	1.70	0.55
1:E:158:PHE:HD1	1:E:462:MET:HE1	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:132:HIS:CG	1:J:222:ILE:CD1	2.89	0.55
1:K:132:HIS:CG	1:K:222:ILE:CD1	2.89	0.55
1:I:620:THR:O	1:I:631:ARG:HG2	2.06	0.55
1:C:100:MET:SD	1:C:109:CYS:HB2	2.46	0.55
1:F:492:SER:O	1:F:493:ASP:HB2	2.05	0.55
1:A:69:ILE:HB	1:A:70:PRO:HD3	1.87	0.55
1:A:132:HIS:CG	1:A:222:ILE:HD12	2.31	0.55
1:E:132:HIS:CD2	1:E:222:ILE:HG12	2.41	0.55
1:G:132:HIS:CD2	1:G:222:ILE:HG12	2.42	0.55
1:G:132:HIS:CG	1:G:222:ILE:CD1	2.89	0.55
1:H:577:ASN:ND2	1:H:635:TYR:OH	2.39	0.55
1:H:132:HIS:CG	1:H:222:ILE:CD1	2.89	0.55
1:L:72:SER:OG	1:L:89:ILE:HD11	2.02	0.55
1:A:94:ILE:O	1:A:98:MET:HB2	2.07	0.55
1:C:348:GLU:O	1:C:348:GLU:HG2	2.06	0.55
1:H:531:LEU:HD12	1:H:532:VAL:N	2.22	0.55
1:J:132:HIS:CD2	1:J:222:ILE:HG12	2.42	0.55
1:K:550:VAL:HG13	1:K:578:PHE:CB	2.37	0.55
1:L:81:LEU:O	1:L:87:ARG:HD2	2.06	0.55
1:L:492:SER:O	1:L:493:ASP:HB2	2.06	0.55
1:A:156:ARG:HA	1:I:279:SER:HB3	1.87	0.55
1:B:64:LEU:HD13	1:B:112:PHE:CD2	2.42	0.55
1:B:319:VAL:HG13	1:B:412:GLU:O	1.98	0.55
1:D:94:ILE:O	1:D:98:MET:HB2	2.07	0.55
1:D:42:GLY:N	1:D:43:PRO:HD2	2.20	0.55
1:L:72:SER:HG	1:L:89:ILE:CD1	2.19	0.55
1:L:348:GLU:HA	1:L:363:HIS:HB3	1.89	0.55
1:C:219:ASN:OD1	1:F:614:VAL:CG2	2.55	0.54
1:D:492:SER:O	1:D:493:ASP:HB2	2.06	0.54
1:F:616:ASP:O	1:F:632:ASP:OD2	2.25	0.54
1:I:621:CYS:HA	1:I:631:ARG:CZ	2.37	0.54
1:C:609:GLU:HG2	1:F:101:ARG:HG2	1.89	0.54
1:G:69:ILE:HB	1:G:70:PRO:HD3	1.90	0.54
1:A:492:SER:O	1:A:493:ASP:HB2	2.06	0.54
1:E:661:THR:OG1	1:E:662:PRO:HD2	2.08	0.54
1:F:349:SER:OG	1:F:361:ASP:CG	2.46	0.54
1:D:615:GLN:NE2	1:D:633:ARG:HB2	2.23	0.54
1:G:492:SER:O	1:G:493:ASP:HB2	2.06	0.54
1:H:132:HIS:CD2	1:H:222:ILE:HG12	2.42	0.54
1:K:132:HIS:CD2	1:K:222:ILE:HG12	2.43	0.54
1:A:132:HIS:CB	1:A:222:ILE:HD12	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:503:PHE:CD1	1:E:645:PHE:HE1	2.26	0.54
1:I:69:ILE:HB	1:I:70:PRO:HD3	1.90	0.54
1:I:492:SER:O	1:I:493:ASP:HB2	2.06	0.54
1:J:268:GLY:HA2	1:J:285:ARG:HH12	1.73	0.54
1:A:132:HIS:CE1	1:A:222:ILE:HD11	2.40	0.54
1:B:633:ARG:NH2	1:D:616:ASP:HB3	2.22	0.54
1:C:69:ILE:HB	1:C:70:PRO:HD3	1.90	0.53
1:E:425:LEU:O	1:E:661:THR:HG21	2.08	0.53
1:C:62:ILE:CD1	1:C:105:GLU:HG2	2.38	0.53
1:E:156:ARG:HA	1:J:279:SER:HB3	1.90	0.53
1:F:98:MET:HE1	1:F:132:HIS:HB3	1.88	0.53
1:L:132:HIS:ND1	1:L:222:ILE:CD1	2.71	0.53
1:L:215:PHE:HB3	1:L:348:GLU:OE1	2.08	0.53
1:I:556:ARG:HD2	1:I:622:ASN:HD21	1.72	0.53
1:J:120:TYR:OH	1:J:150:ASP:OD2	2.24	0.53
1:D:3:TYR:HB3	1:D:103:ILE:HG12	1.90	0.53
1:F:103:ILE:HG23	1:F:103:ILE:O	2.08	0.53
1:G:120:TYR:OH	1:G:150:ASP:OD2	2.24	0.53
1:L:216:GLU:O	1:L:217:ALA:HB2	2.09	0.53
1:C:30:PRO:HD3	1:C:59:VAL:HG13	1.88	0.53
1:A:215:PHE:CE2	1:A:364:ASN:ND2	2.77	0.53
1:F:221:ALA:C	1:F:222:ILE:HG13	2.34	0.53
1:K:242:ARG:NE	1:K:578:PHE:CE2	2.71	0.53
1:K:621:CYS:SG	1:K:622:ASN:ND2	2.81	0.53
1:A:349:SER:O	1:A:356:ARG:NH1	2.42	0.53
1:C:132:HIS:CD2	1:C:222:ILE:HD11	2.44	0.53
1:J:515:MET:CE	1:J:523:PHE:CD2	2.86	0.53
1:B:101:ARG:CB	1:D:494:ALA:HA	2.17	0.53
1:C:83:ILE:O	1:C:87:ARG:HG2	2.09	0.53
1:E:231:LEU:HD21	1:E:579:CYS:CB	2.39	0.53
1:F:98:MET:HE1	1:F:132:HIS:HB2	1.89	0.53
1:L:503:PHE:CD1	1:L:645:PHE:HE2	2.27	0.53
1:E:67:LEU:O	1:E:71:MET:HE3	2.08	0.53
1:E:218:SER:OG	1:E:220:ARG:HG3	2.09	0.53
1:E:552:ILE:CD1	1:E:556:ARG:HB3	2.39	0.53
1:H:145:VAL:HG23	1:H:204:LEU:HD21	1.91	0.53
1:I:552:ILE:HG23	1:I:582:GLY:HA3	1.90	0.53
1:K:348:GLU:HA	1:K:363:HIS:HB3	1.91	0.53
1:L:579:CYS:SG	1:L:627:TYR:CZ	2.99	0.53
1:H:348:GLU:HA	1:H:363:HIS:HB3	1.91	0.52
1:J:581:CYS:SG	1:J:622:ASN:CG	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:PHE:HZ	1:J:167:VAL:HA	1.74	0.52
1:L:221:ALA:C	1:L:222:ILE:HG13	2.34	0.52
1:A:615:GLN:C	1:E:220:ARG:HH21	2.18	0.52
1:C:349:SER:HB2	1:C:361:ASP:HA	1.90	0.52
1:H:69:ILE:HB	1:H:70:PRO:HD3	1.92	0.52
1:I:145:VAL:HG23	1:I:204:LEU:HD21	1.92	0.52
1:L:132:HIS:CD2	1:L:222:ILE:HG12	2.45	0.52
1:C:348:GLU:HG3	1:C:363:HIS:ND1	2.24	0.52
1:D:279:SER:HB3	1:G:156:ARG:HA	1.92	0.52
1:J:145:VAL:HG23	1:J:204:LEU:HD21	1.91	0.52
1:K:145:VAL:HG23	1:K:204:LEU:HD21	1.92	0.52
1:K:69:ILE:HB	1:K:70:PRO:HD3	1.91	0.52
1:L:295:ASN:HB2	4:L:805:HOH:O	2.08	0.52
1:D:60:ARG:CZ	1:D:104:GLU:OE1	2.58	0.52
1:F:348:GLU:HA	1:F:363:HIS:HB3	1.91	0.52
1:H:531:LEU:HD12	1:H:532:VAL:H	1.75	0.52
1:J:231:LEU:HD11	1:J:579:CYS:HB2	1.92	0.52
1:A:423:SER:HB2	1:F:423:SER:OG	2.08	0.52
1:C:145:VAL:HG23	1:C:204:LEU:HD21	1.92	0.52
1:D:349:SER:HB3	1:D:356:ARG:HH11	1.74	0.52
1:E:67:LEU:HB3	1:E:71:MET:CE	2.36	0.52
1:E:304:ASP:OD2	1:F:257:ARG:NH1	2.42	0.52
1:F:92:ARG:NH2	1:F:96:ILE:HD11	2.25	0.52
1:J:218:SER:OG	1:J:220:ARG:HG3	2.10	0.52
1:K:216:GLU:O	1:K:217:ALA:HB2	2.09	0.52
1:C:94:ILE:HD13	1:C:128:VAL:CB	2.40	0.52
1:E:221:ALA:C	1:E:222:ILE:HG13	2.34	0.52
1:G:37:ARG:HD2	1:G:37:ARG:O	2.10	0.52
1:D:281:THR:HG23	1:G:281:THR:HG23	1.91	0.52
1:E:216:GLU:O	1:E:217:ALA:HB2	2.10	0.52
1:E:552:ILE:CD1	1:E:556:ARG:HG2	2.40	0.52
1:J:579:CYS:N	1:J:627:TYR:CE2	2.78	0.52
1:C:279:SER:HB3	1:H:156:ARG:HA	1.92	0.52
1:K:620:THR:CB	1:K:629:GLY:C	2.83	0.52
1:D:85:ARG:O	1:D:88:LYS:HG2	2.10	0.51
1:F:145:VAL:HG23	1:F:204:LEU:HD21	1.91	0.51
1:H:132:HIS:CG	1:H:222:ILE:HG12	2.45	0.51
1:C:609:GLU:OE1	1:F:101:ARG:HD3	2.09	0.51
1:E:145:VAL:HG23	1:E:204:LEU:HD21	1.91	0.51
1:E:192:ARG:NH1	1:E:251:ARG:NE	2.57	0.51
1:J:216:GLU:O	1:J:217:ALA:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:PHE:CE1	1:F:333:PHE:CD1	2.98	0.51
1:G:556:ARG:HD2	1:G:622:ASN:HD21	1.76	0.51
1:K:620:THR:O	1:K:621:CYS:HB3	2.10	0.51
1:F:3:TYR:HB3	1:F:103:ILE:HG23	1.93	0.51
1:F:216:GLU:O	1:F:217:ALA:HB2	2.10	0.51
1:J:500:VAL:O	1:J:529:LYS:HA	2.11	0.51
1:L:540:ARG:O	1:L:540:ARG:CG	2.54	0.51
1:A:42:GLY:O	1:A:45:ILE:HB	2.09	0.51
1:D:145:VAL:HG23	1:D:204:LEU:HD21	1.91	0.51
1:G:145:VAL:HG23	1:G:204:LEU:HD21	1.92	0.51
1:J:221:ALA:C	1:J:222:ILE:HG13	2.35	0.51
1:A:223:VAL:O	1:A:228:ARG:HD2	2.11	0.51
1:C:79:PHE:O	1:C:86:HIS:CD2	2.63	0.51
1:D:218:SER:OG	1:D:219:ASN:N	2.44	0.51
1:E:478:GLN:NE2	1:E:554:PHE:HZ	2.09	0.51
1:F:459:SER:OG	1:F:468:GLY:O	2.29	0.51
1:G:216:GLU:O	1:G:217:ALA:HB2	2.11	0.51
1:H:221:ALA:C	1:H:222:ILE:HG13	2.34	0.51
1:H:556:ARG:HD2	1:H:622:ASN:HD21	1.74	0.51
1:J:132:HIS:CG	1:J:222:ILE:HG12	2.46	0.51
1:K:500:VAL:O	1:K:529:LYS:HA	2.11	0.51
1:B:146:GLU:OE2	1:B:558:PHE:CE1	2.63	0.51
1:B:500:VAL:O	1:B:529:LYS:HA	2.11	0.51
1:F:3:TYR:HB3	1:F:103:ILE:CG2	2.41	0.51
1:F:500:VAL:O	1:F:529:LYS:HA	2.11	0.51
1:H:497:MET:HE1	1:H:533:ALA:HB2	1.92	0.51
1:H:500:VAL:O	1:H:529:LYS:HA	2.11	0.51
1:I:209:TRP:HD1	1:I:580:GLY:HA3	1.76	0.51
1:I:500:VAL:O	1:I:529:LYS:HA	2.11	0.51
1:J:161:ILE:CG2	1:J:462:MET:HE3	2.40	0.51
1:K:556:ARG:HD2	1:K:622:ASN:HD21	1.76	0.51
1:A:321:GLN:HG3	1:A:323:TYR:CZ	2.45	0.51
1:I:453:GLN:HA	1:I:474:PHE:O	2.11	0.51
1:D:39:ARG:HG2	1:D:39:ARG:HH21	1.75	0.51
1:D:500:VAL:O	1:D:529:LYS:HA	2.11	0.51
1:I:31:ASP:O	1:I:39:ARG:HD3	2.09	0.51
1:L:145:VAL:HG23	1:L:204:LEU:HD21	1.91	0.51
1:L:579:CYS:HA	1:L:627:TYR:CE2	2.46	0.51
1:C:31:ASP:O	1:C:39:ARG:HD3	2.11	0.51
1:D:77:GLU:OE1	1:G:156:ARG:NH2	2.36	0.51
1:D:613:VAL:O	1:D:615:GLN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:500:VAL:O	1:E:529:LYS:HA	2.11	0.51
1:J:69:ILE:HB	1:J:70:PRO:HD3	1.93	0.51
1:K:221:ALA:C	1:K:222:ILE:HG13	2.35	0.51
1:L:453:GLN:HA	1:L:474:PHE:O	2.11	0.51
1:B:223:VAL:O	1:B:228:ARG:HD2	2.11	0.50
1:D:453:GLN:HA	1:D:474:PHE:O	2.11	0.50
1:E:132:HIS:CG	1:E:222:ILE:HG12	2.45	0.50
1:E:453:GLN:HA	1:E:474:PHE:O	2.11	0.50
1:F:93:LEU:HD13	1:F:125:ALA:HB1	1.93	0.50
1:A:145:VAL:HG23	1:A:204:LEU:HD21	1.92	0.50
1:A:217:ALA:HB3	1:A:223:VAL:HG23	1.92	0.50
1:B:156:ARG:HA	1:K:279:SER:HB3	1.93	0.50
1:D:507:LYS:HE3	1:D:668:SER:OG	2.12	0.50
1:G:348:GLU:HA	1:G:363:HIS:HB3	1.92	0.50
1:H:140:ASP:OD2	1:H:559:ARG:CZ	2.60	0.50
1:I:85:ARG:O	1:I:88:LYS:HG2	2.11	0.50
1:L:192:ARG:NH1	1:L:251:ARG:NE	2.59	0.50
1:C:330:ASN:HD22	1:F:332:ILE:CD1	2.25	0.50
1:C:500:VAL:O	1:C:529:LYS:HA	2.11	0.50
1:F:251:ARG:HE	1:J:251:ARG:NE	2.08	0.50
1:G:67:LEU:HB3	1:G:71:MET:HE3	1.93	0.50
1:G:221:ALA:C	1:G:222:ILE:HG13	2.35	0.50
1:J:52:LEU:O	1:J:52:LEU:HD23	2.11	0.50
1:J:453:GLN:HA	1:J:474:PHE:O	2.11	0.50
1:D:140:ASP:CG	1:D:556:ARG:HH22	2.16	0.50
1:E:348:GLU:HA	1:E:363:HIS:HB3	1.93	0.50
1:F:453:GLN:HA	1:F:474:PHE:O	2.11	0.50
1:H:349:SER:OG	1:H:361:ASP:CG	2.47	0.50
1:I:221:ALA:C	1:I:222:ILE:HG12	2.37	0.50
1:J:348:GLU:HA	1:J:363:HIS:HB3	1.93	0.50
1:E:581:CYS:SG	1:E:622:ASN:HB2	2.52	0.50
1:F:132:HIS:CG	1:F:222:ILE:CG1	2.95	0.50
1:F:552:ILE:HD13	1:F:583:TRP:O	2.12	0.50
1:G:62:ILE:HG22	1:G:64:LEU:CD1	2.42	0.50
1:G:62:ILE:HG23	1:G:64:LEU:HD13	1.94	0.50
1:B:353:SER:HB3	1:B:356:ARG:HG2	1.94	0.50
1:E:349:SER:O	1:E:356:ARG:NH1	2.45	0.50
1:E:353:SER:HB3	1:E:356:ARG:HG2	1.93	0.50
1:E:478:GLN:NE2	1:E:554:PHE:CZ	2.80	0.50
1:G:453:GLN:HA	1:G:474:PHE:O	2.11	0.50
1:J:556:ARG:HD2	1:J:622:ASN:HD21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:HIS:ND1	1:E:222:ILE:CD1	2.74	0.50
1:H:216:GLU:O	1:H:217:ALA:HB2	2.11	0.50
1:K:132:HIS:CG	1:K:222:ILE:HG12	2.47	0.50
1:A:321:GLN:NE2	1:A:323:TYR:CE2	2.79	0.50
1:B:145:VAL:HG23	1:B:204:LEU:HD21	1.92	0.50
1:C:156:ARG:HA	1:H:279:SER:HB3	1.94	0.50
1:G:500:VAL:O	1:G:529:LYS:HA	2.11	0.50
1:I:132:HIS:CD2	1:I:222:ILE:HG21	2.47	0.50
1:B:453:GLN:HA	1:B:474:PHE:O	2.11	0.50
1:H:526:GLU:OE2	1:H:577:ASN:HB2	2.11	0.50
1:L:500:VAL:O	1:L:529:LYS:HA	2.11	0.50
1:A:103:ILE:CG2	1:A:103:ILE:O	2.60	0.49
1:C:609:GLU:OE1	1:F:101:ARG:NH1	2.42	0.49
1:F:69:ILE:HB	1:F:70:PRO:HD3	1.94	0.49
1:F:622:ASN:OD1	1:F:629:GLY:CA	2.54	0.49
1:G:621:CYS:SG	1:G:622:ASN:N	2.85	0.49
1:K:238:GLN:HB3	1:K:578:PHE:CE2	2.47	0.49
1:K:453:GLN:HA	1:K:474:PHE:O	2.11	0.49
1:L:556:ARG:HD2	1:L:622:ASN:HD21	1.76	0.49
1:A:453:GLN:HA	1:A:474:PHE:O	2.12	0.49
1:C:223:VAL:O	1:C:228:ARG:HD2	2.12	0.49
1:C:453:GLN:HA	1:C:474:PHE:O	2.11	0.49
1:F:132:HIS:CG	1:F:222:ILE:HD11	2.46	0.49
1:H:132:HIS:ND1	1:H:222:ILE:CD1	2.75	0.49
1:K:132:HIS:ND1	1:K:222:ILE:CD1	2.74	0.49
1:A:459:SER:OG	1:A:468:GLY:O	2.30	0.49
1:B:459:SER:OG	1:B:468:GLY:O	2.30	0.49
1:F:37:ARG:NH2	1:L:164:GLU:OE2	2.46	0.49
1:H:453:GLN:HA	1:H:474:PHE:O	2.11	0.49
1:I:216:GLU:O	1:I:217:ALA:HB2	2.10	0.49
1:J:581:CYS:SG	1:J:622:ASN:OD1	2.70	0.49
1:K:223:VAL:O	1:K:228:ARG:HD2	2.12	0.49
1:A:24:LYS:HB3	1:A:54:GLU:HG3	1.95	0.49
1:A:220:ARG:HB3	1:A:224:ASP:HB2	1.93	0.49
1:B:503:PHE:CD1	1:B:645:PHE:HE1	2.30	0.49
1:D:19:PHE:CZ	1:D:38:TYR:CD2	3.00	0.49
1:F:37:ARG:HD2	1:F:37:ARG:O	2.11	0.49
1:F:353:SER:HB3	1:F:356:ARG:HG2	1.94	0.49
1:D:93:LEU:HD11	1:D:117:ILE:CD1	2.42	0.49
1:J:132:HIS:ND1	1:J:222:ILE:CD1	2.75	0.49
1:A:423:SER:CB	1:F:423:SER:OG	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:VAL:O	1:A:529:LYS:HA	2.11	0.49
1:E:94:ILE:O	1:E:98:MET:HB2	2.13	0.49
1:C:42:GLY:N	1:C:43:PRO:HD2	2.26	0.49
1:C:627:TYR:HE1	1:C:631:ARG:HH12	1.59	0.49
1:D:37:ARG:C	1:D:37:ARG:CD	2.86	0.49
1:D:353:SER:HB3	1:D:356:ARG:HG2	1.94	0.49
1:E:250:ASN:C	1:E:251:ARG:CD	2.85	0.49
1:G:353:SER:HB3	1:G:356:ARG:HG2	1.94	0.49
1:K:620:THR:HG23	1:K:628:CYS:C	2.38	0.49
1:H:503:PHE:CD1	1:H:645:PHE:HE1	2.30	0.49
1:J:26:VAL:CG1	1:J:56:ARG:HG3	2.42	0.49
1:K:218:SER:OG	1:K:220:ARG:HG3	2.13	0.49
1:A:67:LEU:HD12	1:A:96:ILE:CD1	2.42	0.49
1:C:84:PRO:HA	1:C:87:ARG:HG3	1.95	0.49
1:E:92:ARG:HD3	1:E:92:ARG:C	2.38	0.49
1:J:223:VAL:O	1:J:228:ARG:HD2	2.13	0.49
1:A:338:LYS:HZ3	1:E:328:SER:CB	2.25	0.49
1:E:581:CYS:SG	1:E:622:ASN:CB	3.01	0.49
1:J:621:CYS:SG	1:J:622:ASN:N	2.85	0.49
1:L:223:VAL:O	1:L:228:ARG:HD2	2.13	0.49
1:L:349:SER:HG	1:L:361:ASP:HA	1.77	0.49
1:D:212:VAL:HG22	1:D:213:TYR:CE1	2.49	0.48
1:I:67:LEU:HB3	1:I:71:MET:HE3	1.95	0.48
1:L:621:CYS:SG	1:L:622:ASN:N	2.86	0.48
1:A:450:TYR:CE1	1:A:678:VAL:HG21	2.47	0.48
1:B:69:ILE:HB	1:B:70:PRO:HD3	1.94	0.48
1:C:281:THR:HG23	1:H:281:THR:HG23	1.95	0.48
1:K:67:LEU:HB3	1:K:71:MET:HE3	1.94	0.48
1:K:350:SER:C	1:K:352:LEU:N	2.71	0.48
1:L:132:HIS:CE1	1:L:222:ILE:HD13	2.48	0.48
1:G:459:SER:OG	1:G:468:GLY:O	2.30	0.48
1:I:232:PHE:CZ	1:I:348:GLU:HB3	2.47	0.48
1:I:349:SER:CB	1:I:361:ASP:OD1	2.61	0.48
1:I:621:CYS:SG	1:I:622:ASN:N	2.85	0.48
1:L:44:GLU:N	1:L:44:GLU:OE1	2.46	0.48
1:B:128:VAL:HA	1:B:131:LEU:CD1	2.43	0.48
1:C:615:GLN:HE21	1:C:634:LEU:CG	2.24	0.48
1:E:459:SER:OG	1:E:468:GLY:O	2.30	0.48
1:G:132:HIS:CG	1:G:222:ILE:HG12	2.47	0.48
1:G:350:SER:C	1:G:352:LEU:N	2.71	0.48
1:I:349:SER:HB3	1:I:361:ASP:OD1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD22	1:A:130:LEU:HG	1.96	0.48
1:C:94:ILE:HD13	1:C:128:VAL:CG1	2.43	0.48
1:H:459:SER:OG	1:H:468:GLY:O	2.31	0.48
1:J:349:SER:HG	1:J:361:ASP:HA	1.79	0.48
1:A:348:GLU:HA	1:A:363:HIS:HB3	1.94	0.48
1:C:219:ASN:OD1	1:F:614:VAL:HG23	2.12	0.48
1:E:192:ARG:CZ	1:E:251:ARG:CZ	2.91	0.48
1:F:31:ASP:O	1:F:39:ARG:HD3	2.14	0.48
1:G:44:GLU:N	1:G:44:GLU:OE1	2.46	0.48
1:H:621:CYS:SG	1:H:622:ASN:N	2.85	0.48
1:A:44:GLU:OE1	1:A:44:GLU:N	2.45	0.48
1:D:219:ASN:OD1	1:D:220:ARG:N	2.47	0.48
1:F:350:SER:C	1:F:352:LEU:N	2.71	0.48
1:L:353:SER:HB3	1:L:356:ARG:HG2	1.95	0.48
1:A:353:SER:HB3	1:A:356:ARG:HG2	1.96	0.48
1:E:192:ARG:HH11	1:E:251:ARG:HD3	1.79	0.48
1:E:223:VAL:O	1:E:228:ARG:HD2	2.13	0.48
1:I:44:GLU:N	1:I:44:GLU:OE1	2.46	0.48
1:I:94:ILE:HD13	1:I:128:VAL:HG11	1.94	0.48
1:K:44:GLU:N	1:K:44:GLU:OE1	2.46	0.48
1:L:215:PHE:CD1	1:L:216:GLU:HG3	2.49	0.48
1:B:67:LEU:HB3	1:B:71:MET:HE3	1.96	0.48
1:C:15:ARG:NH1	1:H:159:GLU:OE2	2.43	0.48
1:D:44:GLU:N	1:D:44:GLU:OE1	2.47	0.48
1:E:231:LEU:N	1:E:641:MET:HE1	2.29	0.48
1:G:132:HIS:ND1	1:G:222:ILE:CD1	2.76	0.48
1:G:223:VAL:O	1:G:228:ARG:HD2	2.14	0.48
1:H:223:VAL:O	1:H:228:ARG:HD2	2.14	0.48
1:J:349:SER:OG	1:J:361:ASP:HA	2.14	0.48
1:L:350:SER:C	1:L:352:LEU:N	2.71	0.48
1:A:350:SER:C	1:A:352:LEU:N	2.72	0.48
1:C:67:LEU:HB3	1:C:71:MET:HE3	1.96	0.48
1:C:350:SER:C	1:C:352:LEU:N	2.71	0.48
1:F:132:HIS:NE2	1:F:222:ILE:HG21	2.29	0.48
1:H:581:CYS:CB	1:H:622:ASN:OD1	2.63	0.47
1:J:44:GLU:OE1	1:J:44:GLU:N	2.46	0.47
1:J:67:LEU:HB3	1:J:71:MET:HE3	1.95	0.47
1:K:621:CYS:SG	1:K:622:ASN:N	2.87	0.47
1:L:349:SER:OG	1:L:361:ASP:HA	2.14	0.47
1:D:223:VAL:O	1:D:228:ARG:HD2	2.14	0.47
1:E:44:GLU:OE1	1:E:44:GLU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:ALA:C	1:F:222:ILE:CG1	2.87	0.47
1:J:12:ASP:OD2	1:J:460:ARG:CZ	2.58	0.47
1:A:254:ARG:CB	1:A:254:ARG:NH1	2.76	0.47
1:B:557:THR:O	1:B:558:PHE:C	2.56	0.47
1:C:459:SER:OG	1:C:468:GLY:O	2.30	0.47
1:H:218:SER:OG	1:H:220:ARG:HG3	2.14	0.47
1:I:350:SER:C	1:I:352:LEU:N	2.71	0.47
1:I:622:ASN:HA	1:I:631:ARG:HH12	1.79	0.47
1:L:94:ILE:O	1:L:98:MET:HB2	2.13	0.47
1:B:81:LEU:HD12	1:B:81:LEU:H	1.80	0.47
1:B:553:PRO:HD2	1:B:556:ARG:HG3	1.96	0.47
1:F:3:TYR:CB	1:F:103:ILE:CG2	2.92	0.47
1:I:209:TRP:CD1	1:I:580:GLY:HA3	2.49	0.47
1:A:182:PHE:HE1	1:A:272:LYS:HB2	1.78	0.47
1:F:44:GLU:N	1:F:44:GLU:OE1	2.46	0.47
1:F:70:PRO:HD3	1:F:92:ARG:CG	2.38	0.47
1:I:511:ARG:HH12	1:K:298:LEU:HD23	1.79	0.47
1:I:632:ASP:O	1:I:633:ARG:C	2.58	0.47
1:K:349:SER:HG	1:K:361:ASP:HA	1.80	0.47
1:A:349:SER:HG	1:A:361:ASP:HA	1.80	0.47
1:E:221:ALA:C	1:E:222:ILE:CG1	2.87	0.47
1:F:218:SER:OG	1:F:220:ARG:HG3	2.14	0.47
1:I:459:SER:OG	1:I:468:GLY:O	2.30	0.47
1:J:161:ILE:HD13	1:J:462:MET:HE2	1.96	0.47
1:A:633:ARG:HD2	1:A:633:ARG:HA	1.51	0.47
1:A:678:VAL:CG1	1:A:679:PRO:HD2	2.20	0.47
1:B:349:SER:OG	1:B:361:ASP:HA	2.14	0.47
1:C:353:SER:HB3	1:C:356:ARG:HG2	1.96	0.47
1:E:92:ARG:HG2	1:E:92:ARG:NH2	2.29	0.47
1:E:192:ARG:NH1	1:E:251:ARG:HD3	2.29	0.47
1:E:620:THR:OG1	1:E:631:ARG:HB2	2.15	0.47
1:G:221:ALA:C	1:G:222:ILE:CG1	2.88	0.47
1:K:253:GLN:OE1	1:K:510:GLU:OE2	2.33	0.47
1:K:459:SER:OG	1:K:468:GLY:O	2.30	0.47
1:K:620:THR:CB	1:K:629:GLY:CA	2.88	0.47
1:H:44:GLU:OE1	1:H:44:GLU:N	2.46	0.47
1:H:304:ASP:OD2	1:K:257:ARG:NH1	2.48	0.47
1:J:353:SER:HB3	1:J:356:ARG:HG2	1.95	0.47
1:A:182:PHE:CE1	1:A:272:LYS:HB2	2.50	0.47
1:A:455:ASP:OD1	1:A:473:ARG:HG2	2.15	0.47
1:F:279:SER:HB3	1:L:156:ARG:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:132:HIS:CG	1:L:222:ILE:HG12	2.50	0.47
1:C:344:GLY:O	1:C:347:ILE:O	2.33	0.47
1:E:70:PRO:CD	1:E:92:ARG:HD2	2.41	0.47
1:G:346:ILE:HG12	1:G:354:PRO:HD2	1.97	0.47
1:L:459:SER:OG	1:L:468:GLY:O	2.30	0.47
1:A:67:LEU:HD12	1:A:70:PRO:HG2	1.97	0.46
1:B:31:ASP:O	1:B:39:ARG:HD3	2.16	0.46
1:K:31:ASP:O	1:K:39:ARG:HD3	2.16	0.46
1:B:279:SER:HB3	1:K:156:ARG:HA	1.97	0.46
1:D:455:ASP:OD1	1:D:473:ARG:HG2	2.15	0.46
1:E:455:ASP:OD1	1:E:473:ARG:HG2	2.16	0.46
1:H:350:SER:C	1:H:352:LEU:N	2.71	0.46
1:J:454:SER:CB	1:J:680:ARG:HD3	2.45	0.46
1:K:353:SER:HB3	1:K:356:ARG:HG2	1.97	0.46
1:K:455:ASP:OD1	1:K:473:ARG:HG2	2.16	0.46
1:L:579:CYS:SG	1:L:579:CYS:O	2.73	0.46
1:C:44:GLU:O	1:C:44:GLU:HG3	2.15	0.46
1:E:20:MET:HE1	1:E:464:PHE:HE1	1.80	0.46
1:E:24:LYS:CD	1:E:54:GLU:OE2	2.63	0.46
1:E:350:SER:C	1:E:352:LEU:N	2.72	0.46
1:H:94:ILE:O	1:H:98:MET:HB2	2.16	0.46
1:A:144:VAL:HA	1:A:147:VAL:HG22	1.98	0.46
1:F:100:MET:O	1:F:133:ARG:CZ	2.55	0.46
1:F:100:MET:HA	1:F:100:MET:CE	2.45	0.46
1:H:221:ALA:C	1:H:222:ILE:CG1	2.88	0.46
1:I:94:ILE:O	1:I:98:MET:HB2	2.15	0.46
1:I:217:ALA:O	1:I:218:SER:OG	2.26	0.46
1:J:509:ASP:OD1	1:J:511:ARG:N	2.38	0.46
1:J:632:ASP:O	1:J:633:ARG:C	2.59	0.46
1:L:192:ARG:CZ	1:L:251:ARG:CZ	2.94	0.46
1:L:250:ASN:C	1:L:251:ARG:HG3	2.39	0.46
1:A:497:MET:HE1	1:A:533:ALA:HB2	1.96	0.46
1:C:503:PHE:CD1	1:C:645:PHE:HE1	2.34	0.46
1:F:126:LEU:HD22	1:F:130:LEU:HG	1.96	0.46
1:G:621:CYS:SG	1:G:622:ASN:ND2	2.89	0.46
1:A:103:ILE:O	1:A:103:ILE:HG23	2.15	0.46
1:B:44:GLU:N	1:B:44:GLU:OE1	2.46	0.46
1:D:643:PHE:HB3	1:D:644:PRO:HD3	1.98	0.46
1:G:497:MET:HE1	1:G:533:ALA:HB2	1.98	0.46
1:G:632:ASP:O	1:G:633:ARG:C	2.59	0.46
1:I:221:ALA:C	1:I:222:ILE:CG1	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:497:MET:HE1	1:J:533:ALA:HB2	1.97	0.46
1:D:19:PHE:HZ	1:D:38:TYR:HD2	1.61	0.46
1:F:67:LEU:HB3	1:F:71:MET:HE3	1.97	0.46
1:H:31:ASP:O	1:H:39:ARG:HD3	2.16	0.46
1:I:579:CYS:H	1:I:627:TYR:HE2	1.62	0.46
1:A:67:LEU:HD13	1:A:96:ILE:HD13	1.94	0.46
1:A:615:GLN:NE2	1:A:633:ARG:HB3	2.31	0.46
1:D:156:ARG:HA	1:G:279:SER:HB3	1.97	0.46
1:I:132:HIS:CG	1:I:222:ILE:HG13	2.50	0.46
1:I:579:CYS:HB2	1:I:627:TYR:OH	2.15	0.46
1:K:94:ILE:O	1:K:98:MET:HB2	2.15	0.46
1:L:31:ASP:O	1:L:39:ARG:HD3	2.15	0.46
1:B:349:SER:HB2	1:B:361:ASP:OD1	2.16	0.46
1:E:661:THR:OG1	1:E:662:PRO:CD	2.64	0.46
1:I:503:PHE:CD1	1:I:645:PHE:HE1	2.34	0.46
1:I:621:CYS:SG	1:I:622:ASN:ND2	2.89	0.46
1:J:221:ALA:C	1:J:222:ILE:CG1	2.88	0.46
1:K:221:ALA:C	1:K:222:ILE:CG1	2.88	0.46
1:K:620:THR:CB	1:K:631:ARG:H	2.29	0.46
1:E:292:LYS:HA	1:E:292:LYS:HE2	1.98	0.46
1:H:621:CYS:SG	1:H:622:ASN:ND2	2.89	0.46
1:L:80:SER:OG	1:L:388:GLY:O	2.31	0.46
1:B:350:SER:C	1:B:352:LEU:N	2.73	0.45
1:E:126:LEU:HD22	1:E:130:LEU:HG	1.98	0.45
1:E:497:MET:HE1	1:E:533:ALA:HB2	1.97	0.45
1:G:511:ARG:NH2	1:J:297:GLU:OE1	2.49	0.45
1:H:94:ILE:HD13	1:H:128:VAL:HG11	1.98	0.45
1:B:98:MET:HE1	1:B:132:HIS:CB	2.46	0.45
1:C:11:TYR:CZ	1:C:141:LEU:CD2	2.99	0.45
1:C:100:MET:O	1:C:133:ARG:NH2	2.49	0.45
1:D:459:SER:OG	1:D:468:GLY:O	2.30	0.45
1:E:93:LEU:HD11	1:E:117:ILE:CD1	2.45	0.45
1:I:93:LEU:HD13	1:I:125:ALA:CB	2.46	0.45
1:J:94:ILE:O	1:J:98:MET:HB2	2.15	0.45
1:J:579:CYS:N	1:J:627:TYR:HE2	2.14	0.45
1:K:632:ASP:O	1:K:633:ARG:C	2.59	0.45
1:L:221:ALA:C	1:L:222:ILE:CG1	2.88	0.45
1:D:454:SER:CB	1:D:554:PHE:HZ	2.29	0.45
1:D:497:MET:HE1	1:D:533:ALA:HB2	1.99	0.45
1:G:680:ARG:HG2	1:G:680:ARG:NH2	2.30	0.45
1:A:614:VAL:HG23	1:E:220:ARG:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:632:ASP:O	1:F:633:ARG:C	2.59	0.45
1:G:94:ILE:O	1:G:98:MET:HB2	2.16	0.45
1:G:639:LYS:HD2	1:G:643:PHE:CE1	2.52	0.45
1:I:350:SER:C	1:I:352:LEU:H	2.25	0.45
1:J:226:ASP:CG	1:J:634:LEU:HD13	2.42	0.45
1:J:346:ILE:HG12	1:J:354:PRO:HD2	1.98	0.45
1:J:639:LYS:HD2	1:J:643:PHE:CE1	2.51	0.45
1:L:222:ILE:HA	1:L:225:LYS:NZ	2.32	0.45
1:L:621:CYS:SG	1:L:622:ASN:ND2	2.89	0.45
1:A:279:SER:HB3	1:I:156:ARG:HA	1.99	0.45
1:B:552:ILE:CG2	1:B:582:GLY:HA3	2.44	0.45
1:C:631:ARG:HA	1:C:631:ARG:HD3	1.53	0.45
1:G:31:ASP:O	1:G:39:ARG:HD3	2.16	0.45
1:G:226:ASP:CG	1:G:634:LEU:HD13	2.41	0.45
1:H:556:ARG:O	1:H:559:ARG:HG2	2.17	0.45
1:J:350:SER:C	1:J:352:LEU:N	2.72	0.45
1:A:200:ILE:HG12	1:A:474:PHE:CE1	2.52	0.45
1:C:107:GLN:O	1:C:111:VAL:HG23	2.17	0.45
1:E:632:ASP:O	1:E:633:ARG:C	2.59	0.45
1:K:350:SER:C	1:K:352:LEU:H	2.25	0.45
1:K:620:THR:CB	1:K:630:VAL:N	2.80	0.45
1:D:212:VAL:CG2	1:D:213:TYR:CE1	3.00	0.45
1:I:497:MET:HE1	1:I:533:ALA:HB2	1.98	0.45
1:J:93:LEU:HD13	1:J:125:ALA:CB	2.47	0.45
1:J:621:CYS:SG	1:J:622:ASN:ND2	2.89	0.45
1:K:226:ASP:CG	1:K:634:LEU:HD13	2.42	0.45
1:L:632:ASP:O	1:L:633:ARG:C	2.59	0.45
1:A:164:GLU:HG3	1:A:173:ARG:HG3	1.98	0.45
1:B:135:ASP:N	1:B:135:ASP:OD1	2.50	0.45
1:F:139:LEU:HD12	1:F:139:LEU:HA	1.84	0.45
1:H:632:ASP:O	1:H:633:ARG:C	2.59	0.45
1:I:80:SER:OG	1:I:388:GLY:O	2.30	0.45
1:I:343:LEU:O	1:I:347:ILE:HG13	2.17	0.45
1:K:94:ILE:HD13	1:K:128:VAL:HG11	1.99	0.45
1:A:3:TYR:CB	1:A:103:ILE:CG2	2.95	0.45
1:B:349:SER:HG	1:B:361:ASP:HA	1.81	0.45
1:D:93:LEU:HD13	1:D:125:ALA:CB	2.46	0.45
1:E:250:ASN:O	1:E:251:ARG:CD	2.47	0.45
1:K:126:LEU:HD22	1:K:130:LEU:HG	1.99	0.45
1:D:19:PHE:CZ	1:D:38:TYR:HD2	2.35	0.44
1:J:126:LEU:HD22	1:J:130:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:144:VAL:HA	1:K:147:VAL:HG22	1.99	0.44
1:L:144:VAL:HA	1:L:147:VAL:HG22	2.00	0.44
1:A:349:SER:OG	1:A:361:ASP:HA	2.16	0.44
1:B:357:GLN:HG2	1:C:416:LYS:NZ	2.32	0.44
1:H:64:LEU:HD22	1:H:109:CYS:HA	1.98	0.44
1:I:117:ILE:CD1	1:I:122:PHE:HB2	2.42	0.44
1:I:418:PRO:O	1:I:647:ARG:HD3	2.17	0.44
1:J:31:ASP:O	1:J:39:ARG:HD3	2.16	0.44
1:K:620:THR:OG1	1:K:630:VAL:N	2.45	0.44
1:L:349:SER:HB3	1:L:356:ARG:NH1	2.31	0.44
1:L:455:ASP:OD1	1:L:473:ARG:HG2	2.17	0.44
1:C:144:VAL:HA	1:C:147:VAL:HG22	2.00	0.44
1:C:497:MET:HE1	1:C:533:ALA:HB2	1.99	0.44
1:D:231:LEU:HD11	1:D:629:GLY:CA	2.46	0.44
1:L:126:LEU:HD22	1:L:130:LEU:HG	2.00	0.44
1:B:349:SER:HB3	1:B:356:ARG:NH1	2.32	0.44
1:F:131:LEU:N	1:F:131:LEU:HD23	2.32	0.44
1:F:556:ARG:HA	1:F:556:ARG:HD3	1.68	0.44
1:H:93:LEU:HD13	1:H:125:ALA:CB	2.47	0.44
1:H:126:LEU:HD22	1:H:130:LEU:HG	1.99	0.44
1:J:455:ASP:OD1	1:J:473:ARG:HG2	2.17	0.44
1:E:93:LEU:HD13	1:E:125:ALA:CB	2.47	0.44
1:G:62:ILE:HG22	1:G:64:LEU:HD13	2.00	0.44
1:G:93:LEU:HD13	1:G:125:ALA:CB	2.48	0.44
1:A:212:VAL:HG22	1:A:213:TYR:CD1	2.52	0.44
1:C:82:PHE:C	1:C:87:ARG:HH21	2.25	0.44
1:F:350:SER:C	1:F:352:LEU:H	2.25	0.44
1:G:350:SER:C	1:G:352:LEU:H	2.25	0.44
1:I:610:ASP:O	1:I:638:ARG:HD3	2.18	0.44
1:J:144:VAL:HA	1:J:147:VAL:HG22	1.99	0.44
1:K:93:LEU:HD13	1:K:125:ALA:CB	2.48	0.44
1:D:129:ALA:O	1:D:133:ARG:HB2	2.18	0.44
1:F:552:ILE:HD13	1:F:552:ILE:N	2.25	0.44
1:K:349:SER:OG	1:K:361:ASP:HA	2.17	0.44
1:B:334:LEU:HD13	1:B:343:LEU:HD11	2.00	0.44
1:D:350:SER:C	1:D:352:LEU:N	2.72	0.44
1:E:280:ARG:HB2	4:E:809:HOH:O	2.16	0.44
1:H:552:ILE:CG2	1:H:582:GLY:HA3	2.48	0.44
1:A:124:TYR:O	1:A:128:VAL:HG23	2.17	0.44
1:C:280:ARG:NH2	1:H:154:ASP:OD2	2.51	0.44
1:E:164:GLU:HG3	1:E:173:ARG:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:661:THR:CG2	1:E:664:MET:CE	2.95	0.44
1:J:350:SER:C	1:J:352:LEU:H	2.26	0.44
1:L:232:PHE:CZ	1:L:348:GLU:HB2	2.53	0.44
1:F:127:SER:O	1:F:129:ALA:N	2.51	0.43
1:F:497:MET:HE1	1:F:533:ALA:HB2	2.00	0.43
1:I:144:VAL:HA	1:I:147:VAL:HG22	1.99	0.43
1:A:357:GLN:HG2	1:B:416:LYS:NZ	2.33	0.43
1:B:163:GLU:HG3	1:K:464:PHE:CZ	2.53	0.43
1:C:24:LYS:HD3	1:C:54:GLU:OE1	2.17	0.43
1:C:455:ASP:OD1	1:C:473:ARG:HG2	2.17	0.43
1:D:43:PRO:HG2	1:D:44:GLU:OE1	2.18	0.43
1:E:144:VAL:HA	1:E:147:VAL:HG22	2.00	0.43
1:G:94:ILE:HD13	1:G:128:VAL:HG11	2.00	0.43
1:H:257:ARG:NH2	1:H:259:ASN:HD22	2.15	0.43
1:H:350:SER:C	1:H:352:LEU:H	2.25	0.43
1:I:544:ARG:HG2	4:I:802:HOH:O	2.18	0.43
1:J:343:LEU:O	1:J:347:ILE:HG13	2.18	0.43
1:L:497:MET:HE1	1:L:533:ALA:HB2	2.00	0.43
1:B:7:LEU:HD11	1:B:103:ILE:CD1	2.48	0.43
1:C:350:SER:C	1:C:352:LEU:H	2.26	0.43
1:D:126:LEU:HD22	1:D:130:LEU:HG	2.00	0.43
1:F:107:GLN:O	1:F:111:VAL:HG23	2.18	0.43
1:F:454:SER:HA	1:F:680:ARG:HD3	1.99	0.43
1:G:107:GLN:O	1:G:111:VAL:HG23	2.18	0.43
1:H:107:GLN:O	1:H:111:VAL:HG23	2.18	0.43
1:H:144:VAL:HA	1:H:147:VAL:HG22	2.00	0.43
1:K:343:LEU:O	1:K:347:ILE:HG13	2.19	0.43
1:L:226:ASP:CG	1:L:634:LEU:HD13	2.42	0.43
1:L:349:SER:HB2	1:L:361:ASP:OD1	2.18	0.43
1:A:93:LEU:HD11	1:A:117:ILE:CD1	2.49	0.43
1:B:343:LEU:O	1:B:347:ILE:HG13	2.18	0.43
1:C:93:LEU:HD11	1:C:117:ILE:CD1	2.49	0.43
1:D:346:ILE:HG12	1:D:354:PRO:HD2	1.99	0.43
1:E:350:SER:C	1:E:352:LEU:H	2.26	0.43
1:F:232:PHE:CZ	1:F:348:GLU:HB2	2.54	0.43
1:I:126:LEU:HD22	1:I:130:LEU:HG	2.00	0.43
1:K:497:MET:HE1	1:K:533:ALA:HB2	1.99	0.43
1:A:678:VAL:CG1	1:A:679:PRO:HD3	2.43	0.43
1:B:107:GLN:O	1:B:111:VAL:HG23	2.18	0.43
1:F:156:ARG:HA	1:L:279:SER:HB3	1.99	0.43
1:H:226:ASP:CG	1:H:634:LEU:HD13	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:ILE:HD13	1:J:128:VAL:HG11	1.99	0.43
1:L:350:SER:C	1:L:352:LEU:H	2.25	0.43
1:C:87:ARG:HG2	1:C:87:ARG:H	1.66	0.43
1:C:132:HIS:CD2	1:C:222:ILE:CD1	3.01	0.43
1:D:37:ARG:NH1	1:G:164:GLU:CD	2.76	0.43
1:D:107:GLN:O	1:D:111:VAL:HG23	2.18	0.43
1:H:350:SER:O	1:H:352:LEU:N	2.52	0.43
1:K:295:ASN:HD22	1:K:302:LYS:HD3	1.83	0.43
1:E:209:TRP:CD1	1:E:580:GLY:HA3	2.54	0.43
1:L:107:GLN:O	1:L:111:VAL:HG23	2.19	0.43
1:F:226:ASP:CG	1:F:634:LEU:HD13	2.43	0.43
1:F:350:SER:O	1:F:352:LEU:N	2.52	0.43
1:H:579:CYS:H	1:H:627:TYR:HE2	1.65	0.43
1:I:455:ASP:OD1	1:I:473:ARG:HG2	2.19	0.43
1:L:94:ILE:HD13	1:L:128:VAL:HG11	2.00	0.43
1:A:254:ARG:HH11	1:A:254:ARG:HB2	1.79	0.43
1:A:639:LYS:HD2	1:A:643:PHE:CE1	2.54	0.43
1:B:94:ILE:HD13	1:B:128:VAL:HG11	2.00	0.43
1:B:558:PHE:C	1:B:558:PHE:CD1	2.97	0.43
1:D:639:LYS:HD2	1:D:643:PHE:CE1	2.53	0.43
1:E:223:VAL:HG11	1:E:351:ILE:HG12	2.00	0.43
1:E:552:ILE:HD12	1:E:556:ARG:CG	2.47	0.43
1:F:62:ILE:HG22	1:F:63:ALA:N	2.33	0.43
1:F:343:LEU:O	1:F:347:ILE:HG13	2.19	0.43
1:G:164:GLU:HG3	1:G:173:ARG:HG3	2.00	0.43
1:H:238:GLN:HB3	1:H:578:PHE:CZ	2.54	0.43
1:I:67:LEU:HD12	1:I:96:ILE:HD13	2.01	0.43
1:J:349:SER:HB2	1:J:361:ASP:OD1	2.19	0.43
1:B:129:ALA:O	1:B:133:ARG:HB2	2.19	0.43
1:B:455:ASP:OD1	1:B:473:ARG:HG2	2.18	0.43
1:C:15:ARG:HD3	1:C:277:VAL:HA	2.01	0.43
1:E:26:VAL:CG1	1:E:56:ARG:HD2	2.48	0.43
1:F:144:VAL:HA	1:F:147:VAL:HG22	2.01	0.43
1:H:455:ASP:OD1	1:H:473:ARG:HG2	2.19	0.43
1:H:577:ASN:CA	1:H:627:TYR:HH	2.31	0.43
1:I:222:ILE:HG22	1:I:222:ILE:O	2.18	0.43
1:J:107:GLN:O	1:J:111:VAL:HG23	2.19	0.43
1:J:349:SER:HB3	1:J:356:ARG:NH1	2.34	0.43
1:A:331:ARG:NH1	1:F:330:ASN:HB3	2.34	0.42
1:D:144:VAL:HA	1:D:147:VAL:HG22	2.01	0.42
1:E:20:MET:HE1	1:E:464:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:THR:HG23	1:J:281:THR:HG23	2.01	0.42
1:E:661:THR:OG1	1:E:662:PRO:N	2.51	0.42
1:G:64:LEU:HD13	1:G:64:LEU:N	2.34	0.42
1:H:491:THR:O	1:H:491:THR:OG1	2.37	0.42
1:K:350:SER:O	1:K:352:LEU:N	2.52	0.42
1:A:18:ILE:HD13	1:A:111:VAL:HG13	2.00	0.42
1:D:257:ARG:NH1	1:F:304:ASP:OD2	2.52	0.42
1:F:212:VAL:HG22	1:F:213:TYR:CD2	2.54	0.42
1:H:629:GLY:O	1:H:630:VAL:CG2	2.66	0.42
1:I:164:GLU:HG3	1:I:173:ARG:HG3	2.01	0.42
1:K:427:TYR:OH	1:K:497:MET:O	2.30	0.42
1:L:67:LEU:HB3	1:L:71:MET:HE3	2.01	0.42
1:B:552:ILE:HD11	1:B:557:THR:HG23	2.01	0.42
1:E:107:GLN:O	1:E:111:VAL:HG23	2.18	0.42
1:F:131:LEU:N	1:F:131:LEU:CD2	2.82	0.42
1:G:93:LEU:HD11	1:G:117:ILE:CD1	2.49	0.42
1:G:126:LEU:HD22	1:G:130:LEU:HG	2.01	0.42
1:G:144:VAL:HA	1:G:147:VAL:HG22	2.00	0.42
1:J:12:ASP:CG	1:J:460:ARG:NH1	2.72	0.42
1:K:132:HIS:CE1	1:K:222:ILE:HD13	2.55	0.42
1:D:350:SER:C	1:D:352:LEU:H	2.27	0.42
1:E:230:GLU:C	1:E:641:MET:HE3	2.44	0.42
1:E:343:LEU:O	1:E:347:ILE:HG13	2.19	0.42
1:G:300:GLN:HG2	1:L:518:ARG:NH1	2.34	0.42
1:H:67:LEU:HB3	1:H:71:MET:HE3	2.00	0.42
1:K:107:GLN:O	1:K:111:VAL:HG23	2.19	0.42
1:L:132:HIS:CG	1:L:222:ILE:HD11	2.53	0.42
1:B:232:PHE:CZ	1:B:348:GLU:HB2	2.54	0.42
1:B:492:SER:O	1:B:493:ASP:CB	2.68	0.42
1:C:32:ASN:OD1	1:C:32:ASN:N	2.44	0.42
1:C:62:ILE:HD13	1:C:105:GLU:HG2	2.01	0.42
1:C:164:GLU:HG3	1:C:173:ARG:HG3	2.01	0.42
1:I:629:GLY:O	1:I:630:VAL:CG2	2.67	0.42
1:J:222:ILE:O	1:J:222:ILE:HG22	2.19	0.42
1:J:552:ILE:CG2	1:J:582:GLY:HA3	2.49	0.42
1:L:164:GLU:HG3	1:L:173:ARG:HG3	2.02	0.42
1:B:386:VAL:HG22	1:B:392:THR:HB	2.02	0.42
1:C:94:ILE:HD13	1:C:128:VAL:HG11	2.02	0.42
1:C:552:ILE:CG2	1:C:582:GLY:HA3	2.49	0.42
1:D:492:SER:O	1:D:493:ASP:CB	2.68	0.42
1:G:18:ILE:HD13	1:G:111:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:455:ASP:OD1	1:G:473:ARG:HG2	2.20	0.42
1:H:18:ILE:HD13	1:H:111:VAL:HG13	2.00	0.42
1:H:232:PHE:CZ	1:H:348:GLU:HB2	2.54	0.42
1:H:343:LEU:O	1:H:347:ILE:HG13	2.18	0.42
1:I:132:HIS:CE1	1:I:222:ILE:HG21	2.54	0.42
1:J:18:ILE:HD13	1:J:111:VAL:HG13	2.02	0.42
1:K:254:ARG:HH11	1:K:254:ARG:CG	2.33	0.42
1:L:492:SER:O	1:L:493:ASP:CB	2.68	0.42
1:A:281:THR:HG23	1:I:281:THR:HG23	2.01	0.42
1:B:144:VAL:HA	1:B:147:VAL:HG22	2.01	0.42
1:C:79:PHE:O	1:C:86:HIS:HD2	2.03	0.42
1:C:223:VAL:HG11	1:C:351:ILE:HG12	2.00	0.42
1:D:152:TYR:HB3	1:D:200:ILE:CD1	2.50	0.42
1:D:164:GLU:HG3	1:D:173:ARG:HG3	2.01	0.42
1:E:18:ILE:HD13	1:E:111:VAL:HG13	2.01	0.42
1:E:132:HIS:CE1	1:E:222:ILE:HD13	2.54	0.42
1:E:279:SER:HB3	1:J:156:ARG:HA	2.00	0.42
1:H:64:LEU:HD13	1:H:112:PHE:CD2	2.54	0.42
1:L:18:ILE:HD13	1:L:111:VAL:HG13	2.02	0.42
1:L:253:GLN:NE2	1:L:254:ARG:O	2.52	0.42
1:A:386:VAL:HG22	1:A:392:THR:HB	2.02	0.42
1:F:222:ILE:HG22	1:F:222:ILE:O	2.19	0.42
1:G:222:ILE:HG22	1:G:222:ILE:O	2.20	0.42
1:J:492:SER:O	1:J:493:ASP:CB	2.68	0.42
1:K:18:ILE:HD13	1:K:111:VAL:HG13	2.02	0.42
1:K:492:SER:O	1:K:493:ASP:CB	2.68	0.42
1:L:222:ILE:O	1:L:222:ILE:HG22	2.20	0.42
1:A:100:MET:O	1:A:133:ARG:NH1	2.46	0.42
1:B:281:THR:HG23	1:K:281:THR:HG23	2.02	0.42
1:B:350:SER:C	1:B:352:LEU:H	2.28	0.42
1:C:18:ILE:HD13	1:C:111:VAL:HG13	2.02	0.42
1:C:34:LEU:CD2	1:C:46:GLN:HE22	2.32	0.42
1:C:348:GLU:CG	1:C:363:HIS:HD1	2.31	0.42
1:D:212:VAL:CG2	1:D:213:TYR:CD1	2.98	0.42
1:D:454:SER:HG	1:D:554:PHE:HE2	1.67	0.42
1:E:94:ILE:HD13	1:E:128:VAL:HG11	2.00	0.42
1:G:350:SER:O	1:G:352:LEU:N	2.51	0.42
1:G:554:PHE:CD2	1:G:680:ARG:NH2	2.88	0.42
1:H:577:ASN:N	1:H:627:TYR:OH	2.53	0.42
1:I:222:ILE:HD13	1:I:222:ILE:N	2.35	0.42
1:I:492:SER:O	1:I:493:ASP:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:232:PHE:CZ	1:J:348:GLU:HB2	2.55	0.42
1:K:232:PHE:CZ	1:K:348:GLU:HB2	2.55	0.42
1:L:84:PRO:HG2	1:L:300:GLN:O	2.20	0.42
1:B:214:PRO:O	1:B:223:VAL:HG13	2.19	0.42
1:D:350:SER:O	1:D:352:LEU:N	2.52	0.42
1:F:15:ARG:HD3	1:F:277:VAL:HA	2.01	0.42
1:F:18:ILE:HD13	1:F:111:VAL:HG13	2.01	0.42
1:H:222:ILE:HG22	1:H:222:ILE:O	2.19	0.42
1:L:350:SER:O	1:L:352:LEU:N	2.53	0.42
1:L:629:GLY:O	1:L:630:VAL:CG2	2.66	0.42
1:A:350:SER:C	1:A:352:LEU:H	2.26	0.41
1:A:357:GLN:HE21	1:B:320:HIS:HD2	1.68	0.41
1:B:346:ILE:HG12	1:B:354:PRO:HD2	2.02	0.41
1:B:411:GLN:C	1:B:413:HIS:H	2.28	0.41
1:C:103:ILE:HD12	1:C:103:ILE:O	2.20	0.41
1:C:126:LEU:HD22	1:C:130:LEU:HG	2.01	0.41
1:D:37:ARG:HB3	1:D:38:TYR:HD1	1.85	0.41
1:E:492:SER:O	1:E:493:ASP:CB	2.67	0.41
1:F:175:PRO:HG2	1:F:473:ARG:CZ	2.50	0.41
1:F:552:ILE:CD1	1:F:582:GLY:C	2.87	0.41
1:A:492:SER:O	1:A:493:ASP:CB	2.67	0.41
1:C:80:SER:HB2	1:C:384:PHE:CZ	2.55	0.41
1:C:634:LEU:HD22	1:C:634:LEU:HA	1.79	0.41
1:D:60:ARG:NH1	1:D:104:GLU:CD	2.77	0.41
1:D:67:LEU:HD12	1:D:96:ILE:HD13	2.01	0.41
1:E:192:ARG:NH1	1:E:251:ARG:CD	2.84	0.41
1:F:69:ILE:HB	1:F:92:ARG:HG2	2.02	0.41
1:G:15:ARG:HD3	1:G:277:VAL:HA	2.02	0.41
1:J:93:LEU:HD11	1:J:117:ILE:CD1	2.50	0.41
1:L:15:ARG:HD3	1:L:277:VAL:HA	2.02	0.41
1:B:93:LEU:HD13	1:B:125:ALA:CB	2.50	0.41
1:B:126:LEU:HD22	1:B:130:LEU:HG	2.02	0.41
1:E:209:TRP:HD1	1:E:580:GLY:HA3	1.84	0.41
1:G:153:VAL:HG11	1:G:157:VAL:HG21	2.02	0.41
1:G:343:LEU:O	1:G:347:ILE:HG13	2.20	0.41
1:H:164:GLU:HG3	1:H:173:ARG:HG3	2.02	0.41
1:A:220:ARG:O	1:A:224:ASP:N	2.49	0.41
1:B:615:GLN:NE2	1:B:633:ARG:CB	2.66	0.41
1:D:37:ARG:HD3	1:D:38:TYR:CD1	2.55	0.41
1:F:492:SER:O	1:F:493:ASP:CB	2.67	0.41
1:L:343:LEU:O	1:L:347:ILE:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLN:O	1:A:111:VAL:HG23	2.20	0.41
1:A:349:SER:HB2	1:A:361:ASP:OD1	2.20	0.41
1:E:216:GLU:O	1:E:217:ALA:CB	2.69	0.41
1:G:232:PHE:CZ	1:G:348:GLU:HB2	2.56	0.41
1:H:526:GLU:OE1	1:H:577:ASN:HB3	2.21	0.41
1:I:107:GLN:O	1:I:111:VAL:HG23	2.19	0.41
1:J:152:TYR:HB3	1:J:200:ILE:HD12	2.02	0.41
1:K:15:ARG:HD3	1:K:277:VAL:HA	2.02	0.41
1:A:215:PHE:HB2	1:A:350:SER:HA	2.02	0.41
1:A:219:ASN:N	1:A:219:ASN:ND2	2.69	0.41
1:A:280:ARG:NH1	1:I:154:ASP:OD1	2.53	0.41
1:A:634:LEU:HD13	1:A:634:LEU:HA	1.95	0.41
1:B:220:ARG:HH12	1:D:638:ARG:HH12	1.68	0.41
1:B:497:MET:HE1	1:B:533:ALA:HB2	2.01	0.41
1:C:350:SER:O	1:C:352:LEU:N	2.53	0.41
1:G:132:HIS:CE1	1:G:222:ILE:HD13	2.55	0.41
1:G:492:SER:O	1:G:493:ASP:CB	2.68	0.41
1:H:132:HIS:CE1	1:H:222:ILE:HD13	2.55	0.41
1:J:350:SER:O	1:J:352:LEU:N	2.54	0.41
1:L:132:HIS:CB	1:L:222:ILE:HD11	2.51	0.41
1:A:152:TYR:HB3	1:A:200:ILE:CD1	2.51	0.41
1:B:18:ILE:HD13	1:B:111:VAL:HG13	2.02	0.41
1:B:164:GLU:HG3	1:B:173:ARG:HG3	2.02	0.41
1:B:350:SER:O	1:B:352:LEU:N	2.54	0.41
1:B:643:PHE:CD1	1:B:643:PHE:C	2.98	0.41
1:D:386:VAL:HG22	1:D:392:THR:HB	2.03	0.41
1:F:164:GLU:HG3	1:F:173:ARG:HG3	2.02	0.41
1:F:216:GLU:O	1:F:217:ALA:CB	2.69	0.41
1:G:62:ILE:CG2	1:G:64:LEU:CD1	2.98	0.41
1:G:80:SER:OG	1:G:388:GLY:O	2.30	0.41
1:H:124:TYR:O	1:H:128:VAL:HG23	2.21	0.41
1:H:153:VAL:HG11	1:H:157:VAL:HG21	2.02	0.41
1:I:348:GLU:O	1:I:348:GLU:HG3	2.21	0.41
1:L:124:TYR:O	1:L:128:VAL:HG23	2.21	0.41
1:A:15:ARG:HD3	1:A:277:VAL:HA	2.02	0.41
1:C:212:VAL:HG22	1:C:213:TYR:CD2	2.56	0.41
1:F:251:ARG:HE	1:J:251:ARG:HE	1.69	0.41
1:F:503:PHE:CD1	1:F:645:PHE:HE1	2.38	0.41
1:L:101:ARG:HD2	1:L:102:ASN:H	1.86	0.41
1:L:152:TYR:HB3	1:L:200:ILE:HD12	2.03	0.41
1:L:152:TYR:HB3	1:L:200:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLU:H	1:B:54:GLU:HG2	1.52	0.41
1:B:212:VAL:HG22	1:B:213:TYR:CD2	2.56	0.41
1:B:639:LYS:HD2	1:B:643:PHE:CE1	2.56	0.41
1:C:343:LEU:O	1:C:347:ILE:HG13	2.20	0.41
1:D:18:ILE:HD13	1:D:111:VAL:HG13	2.03	0.41
1:D:215:PHE:HB2	1:D:350:SER:HA	2.02	0.41
1:F:552:ILE:N	1:F:552:ILE:CD1	2.84	0.41
1:G:216:GLU:O	1:G:217:ALA:CB	2.69	0.41
1:G:223:VAL:HG11	1:G:351:ILE:HG12	2.02	0.41
1:H:15:ARG:HD3	1:H:277:VAL:HA	2.03	0.41
1:H:93:LEU:HD11	1:H:117:ILE:CD1	2.50	0.41
1:I:15:ARG:HD3	1:I:277:VAL:HA	2.02	0.41
1:I:76:GLN:O	1:I:278:ALA:HA	2.21	0.41
1:I:152:TYR:HB3	1:I:200:ILE:CD1	2.51	0.41
1:J:427:TYR:OH	1:J:497:MET:O	2.29	0.41
1:K:93:LEU:HD11	1:K:117:ILE:CD1	2.51	0.41
1:K:152:TYR:HB3	1:K:200:ILE:CD1	2.51	0.41
1:K:164:GLU:HG3	1:K:173:ARG:HG3	2.02	0.41
1:K:216:GLU:O	1:K:217:ALA:CB	2.69	0.41
1:K:349:SER:HB2	1:K:361:ASP:OD1	2.20	0.41
1:K:552:ILE:CG2	1:K:582:GLY:HA3	2.49	0.41
1:K:617:LEU:H	1:K:617:LEU:CD1	2.34	0.41
1:L:212:VAL:HG22	1:L:213:TYR:CD2	2.56	0.41
1:L:552:ILE:CG2	1:L:582:GLY:HA3	2.49	0.41
1:B:93:LEU:HD11	1:B:117:ILE:CD1	2.51	0.41
1:B:124:TYR:O	1:B:128:VAL:HG23	2.21	0.41
1:C:492:SER:O	1:C:493:ASP:CB	2.68	0.41
1:D:219:ASN:OD1	1:D:219:ASN:C	2.62	0.41
1:E:386:VAL:HG22	1:E:392:THR:HB	2.02	0.41
1:L:76:GLN:O	1:L:278:ALA:HA	2.21	0.41
1:B:15:ARG:HD3	1:B:277:VAL:HA	2.03	0.40
1:C:491:THR:O	1:C:491:THR:OG1	2.38	0.40
1:E:350:SER:O	1:E:352:LEU:N	2.54	0.40
1:F:152:TYR:HB3	1:F:200:ILE:CD1	2.51	0.40
1:G:386:VAL:HG22	1:G:392:THR:HB	2.04	0.40
1:I:386:VAL:HG22	1:I:392:THR:HB	2.02	0.40
1:J:124:TYR:O	1:J:128:VAL:HG23	2.21	0.40
1:L:643:PHE:CD1	1:L:643:PHE:C	2.99	0.40
1:B:334:LEU:HD13	1:B:343:LEU:CD1	2.51	0.40
1:C:76:GLN:O	1:C:278:ALA:HA	2.22	0.40
1:D:302:LYS:HZ3	1:E:257:ARG:HD3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:GLN:O	1:F:278:ALA:HA	2.21	0.40
1:H:492:SER:O	1:H:493:ASP:CB	2.68	0.40
1:I:18:ILE:HD13	1:I:111:VAL:HG13	2.02	0.40
1:I:209:TRP:H	1:I:581:CYS:HG	1.69	0.40
1:I:552:ILE:CG2	1:I:582:GLY:HA3	2.49	0.40
1:A:93:LEU:HD13	1:A:125:ALA:CB	2.52	0.40
1:A:350:SER:O	1:A:352:LEU:N	2.54	0.40
1:B:48:ARG:HG2	1:B:48:ARG:HH11	1.86	0.40
1:B:219:ASN:HB3	1:B:222:ILE:HD12	2.03	0.40
1:E:556:ARG:CZ	1:E:621:CYS:SG	3.10	0.40
1:H:386:VAL:HG22	1:H:392:THR:HB	2.03	0.40
1:H:521:ARG:HB2	1:H:645:PHE:HB3	2.04	0.40
1:J:76:GLN:O	1:J:278:ALA:HA	2.21	0.40
1:J:132:HIS:CE1	1:J:222:ILE:HD13	2.55	0.40
1:J:212:VAL:HG22	1:J:213:TYR:CD2	2.56	0.40
1:K:620:THR:OG1	1:K:621:CYS:N	2.54	0.40
1:L:153:VAL:HG11	1:L:157:VAL:HG21	2.04	0.40
1:A:232:PHE:CZ	1:A:348:GLU:HB2	2.56	0.40
1:A:338:LYS:NZ	1:E:328:SER:HB3	2.36	0.40
1:C:39:ARG:N	1:C:40:PRO:CD	2.85	0.40
1:D:15:ARG:HD3	1:D:277:VAL:HA	2.04	0.40
1:I:152:TYR:HB3	1:I:200:ILE:HD12	2.03	0.40
1:D:76:GLN:O	1:D:278:ALA:HA	2.22	0.40
1:E:152:TYR:HB3	1:E:200:ILE:CD1	2.51	0.40
1:E:222:ILE:O	1:E:222:ILE:HG22	2.21	0.40
1:F:552:ILE:HD12	1:F:582:GLY:CA	2.50	0.40
1:F:639:LYS:HD2	1:F:643:PHE:CE1	2.57	0.40
1:G:124:TYR:O	1:G:128:VAL:HG23	2.21	0.40
1:J:152:TYR:HB3	1:J:200:ILE:CD1	2.51	0.40
1:K:639:LYS:HD2	1:K:643:PHE:CE1	2.57	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:GLU:OE2	1:J:444:VAL:CG1[1_655]	1.59	0.61
1:A:47:ASN:OD1	1:C:438:GLN:NE2[1_656]	1.60	0.60
1:G:102:ASN:OD1	1:K:330:ASN:ND2[2_645]	1.95	0.25
1:A:47:ASN:OD1	1:C:438:GLN:CD[1_656]	1.96	0.24
1:H:102:ASN:OD1	1:L:330:ASN:ND2[2_555]	2.03	0.17
1:A:47:ASN:ND2	1:C:483:GLN:OE1[1_656]	2.18	0.02

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	645/681 (95%)	608 (94%)	30 (5%)	7 (1%)	11	39
1	B	639/681 (94%)	602 (94%)	32 (5%)	5 (1%)	16	46
1	C	642/681 (94%)	609 (95%)	27 (4%)	6 (1%)	14	43
1	D	644/681 (95%)	610 (95%)	29 (4%)	5 (1%)	16	46
1	E	655/681 (96%)	620 (95%)	30 (5%)	5 (1%)	16	46
1	F	651/681 (96%)	614 (94%)	29 (4%)	8 (1%)	10	37
1	G	653/681 (96%)	615 (94%)	32 (5%)	6 (1%)	14	43
1	H	655/681 (96%)	616 (94%)	32 (5%)	7 (1%)	11	39
1	I	654/681 (96%)	618 (94%)	30 (5%)	6 (1%)	14	43
1	J	653/681 (96%)	614 (94%)	33 (5%)	6 (1%)	14	43
1	K	654/681 (96%)	617 (94%)	29 (4%)	8 (1%)	10	37
1	L	653/681 (96%)	616 (94%)	31 (5%)	6 (1%)	14	43
All	All	7798/8172 (95%)	7359 (94%)	364 (5%)	75 (1%)	12	41

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	SER
1	B	630	VAL
1	D	614	VAL
1	D	643	PHE
1	E	217	ALA
1	E	222	ILE
1	F	127	SER
1	F	217	ALA
1	F	222	ILE
1	G	217	ALA
1	G	222	ILE
1	H	217	ALA

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Mol	Chain	Res	Type
1	H	222	ILE
1	I	217	ALA
1	I	222	ILE
1	J	217	ALA
1	J	222	ILE
1	K	217	ALA
1	K	222	ILE
1	K	621	CYS
1	L	217	ALA
1	L	222	ILE
1	A	222	ILE
1	A	493	ASP
1	A	632	ASP
1	B	493	ASP
1	C	493	ASP
1	C	632	ASP
1	D	493	ASP
1	E	493	ASP
1	E	633	ARG
1	F	128	VAL
1	F	493	ASP
1	G	493	ASP
1	H	493	ASP
1	I	493	ASP
1	J	493	ASP
1	K	493	ASP
1	L	493	ASP
1	L	581	CYS
1	A	217	ALA
1	I	350	SER
1	A	64	LEU
1	B	64	LEU
1	C	64	LEU
1	C	348	GLU
1	D	64	LEU
1	D	218	SER
1	E	64	LEU
1	F	64	LEU
1	G	64	LEU
1	H	64	LEU
1	I	64	LEU
1	I	349	SER

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Mol	Chain	Res	Type
1	J	64	LEU
1	K	64	LEU
1	L	64	LEU
1	B	219	ASN
1	C	80	SER
1	C	219	ASN
1	H	633	ARG
1	J	633	ARG
1	F	633	ARG
1	A	629	GLY
1	K	618	VAL
1	A	679	PRO
1	F	630	VAL
1	G	351	ILE
1	G	630	VAL
1	H	351	ILE
1	J	630	VAL
1	K	351	ILE
1	K	630	VAL
1	L	630	VAL
1	H	630	VAL

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	585/610 (96%)	520 (89%)	65 (11%)	6	22
1	B	580/610 (95%)	512 (88%)	68 (12%)	5	20
1	C	583/610 (96%)	511 (88%)	72 (12%)	4	19
1	D	585/610 (96%)	526 (90%)	59 (10%)	7	26
1	E	594/610 (97%)	527 (89%)	67 (11%)	5	21
1	F	591/610 (97%)	527 (89%)	64 (11%)	6	23
1	G	592/610 (97%)	535 (90%)	57 (10%)	8	28
1	H	594/610 (97%)	539 (91%)	55 (9%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	593/610 (97%)	530 (89%)	63 (11%)	6	24
1	J	592/610 (97%)	535 (90%)	57 (10%)	8	28
1	K	593/610 (97%)	540 (91%)	53 (9%)	9	30
1	L	592/610 (97%)	531 (90%)	61 (10%)	7	25
All	All	7074/7320 (97%)	6333 (90%)	741 (10%)	6	24

All (741) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	46	GLN
1	A	47	ASN
1	A	51	GLU
1	A	56	ARG
1	A	60	ARG
1	A	62	ILE
1	A	67	LEU
1	A	68	ARG
1	A	69	ILE
1	A	73	LEU
1	A	93	LEU
1	A	101	ARG
1	A	103	ILE
1	A	104	GLU
1	A	105	GLU
1	A	126	LEU
1	A	153	VAL
1	A	173	ARG
1	A	174	MET
1	A	177	VAL
1	A	180	LYS
1	A	191	HIS
1	A	202	VAL
1	A	212	VAL
1	A	222	ILE
1	A	231	LEU
1	A	253	GLN
1	A	254	ARG
1	A	257	ARG
1	A	260	ASN
1	A	280	ARG

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Mol	Chain	Res	Type
1	A	290	VAL
1	A	298	LEU
1	A	302	LYS
1	A	308	LEU
1	A	321	GLN
1	A	349	SER
1	A	386	VAL
1	A	411	GLN
1	A	425	LEU
1	A	426	THR
1	A	459	SER
1	A	483	GLN
1	A	491	THR
1	A	497	MET
1	A	499	PHE
1	A	525	VAL
1	A	539	ASN
1	A	540	ARG
1	A	551	THR
1	A	556	ARG
1	A	559	ARG
1	A	614	VAL
1	A	627	TYR
1	A	630	VAL
1	A	631	ARG
1	A	632	ASP
1	A	633	ARG
1	A	634	LEU
1	A	654	ASP
1	A	660	VAL
1	A	678	VAL
1	A	680	ARG
1	A	681	THR
1	B	34	LEU
1	B	48	ARG
1	B	51	GLU
1	B	52	LEU
1	B	54	GLU
1	B	56	ARG
1	B	59	VAL
1	B	62	ILE
1	B	64	LEU

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Mol	Chain	Res	Type
1	B	67	LEU
1	B	68	ARG
1	B	73	LEU
1	B	81	LEU
1	B	88	LYS
1	B	93	LEU
1	B	101	ARG
1	B	103	ILE
1	B	104	GLU
1	B	126	LEU
1	B	131	LEU
1	B	135	ASP
1	B	137	LYS
1	B	153	VAL
1	B	173	ARG
1	B	174	MET
1	B	177	VAL
1	B	180	LYS
1	B	191	HIS
1	B	202	VAL
1	B	212	VAL
1	B	216	GLU
1	B	225	LYS
1	B	231	LEU
1	B	254	ARG
1	B	256	LYS
1	B	260	ASN
1	B	290	VAL
1	B	298	LEU
1	B	308	LEU
1	B	342	ILE
1	B	343	LEU
1	B	347	ILE
1	B	349	SER
1	B	386	VAL
1	B	425	LEU
1	B	426	THR
1	B	459	SER
1	B	473	ARG
1	B	483	GLN
1	B	491	THR
1	B	497	MET

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Mol	Chain	Res	Type
1	B	499	PHE
1	B	518	ARG
1	B	525	VAL
1	B	540	ARG
1	B	551	THR
1	B	554	PHE
1	B	556	ARG
1	B	557	THR
1	B	614	VAL
1	B	631	ARG
1	B	633	ARG
1	B	651	THR
1	B	654	ASP
1	B	660	VAL
1	B	672	ILE
1	B	680	ARG
1	B	681	THR
1	C	29	VAL
1	C	31	ASP
1	C	34	LEU
1	C	35	THR
1	C	45	ILE
1	C	46	GLN
1	C	49	PHE
1	C	59	VAL
1	C	60	ARG
1	C	62	ILE
1	C	67	LEU
1	C	73	LEU
1	C	87	ARG
1	C	93	LEU
1	C	94	ILE
1	C	98	MET
1	C	100	MET
1	C	103	ILE
1	C	104	GLU
1	C	126	LEU
1	C	137	LYS
1	C	138	ASN
1	C	141	LEU
1	C	153	VAL
1	C	173	ARG

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Mol	Chain	Res	Type
1	C	174	MET
1	C	177	VAL
1	C	180	LYS
1	C	191	HIS
1	C	202	VAL
1	C	212	VAL
1	C	218	SER
1	C	219	ASN
1	C	231	LEU
1	C	251	ARG
1	C	254	ARG
1	C	259	ASN
1	C	260	ASN
1	C	290	VAL
1	C	297	GLU
1	C	298	LEU
1	C	308	LEU
1	C	347	ILE
1	C	348	GLU
1	C	386	VAL
1	C	425	LEU
1	C	426	THR
1	C	459	SER
1	C	473	ARG
1	C	483	GLN
1	C	491	THR
1	C	497	MET
1	C	499	PHE
1	C	507	LYS
1	C	508	ASN
1	C	510	GLU
1	C	511	ARG
1	C	513	GLN
1	C	518	ARG
1	C	525	VAL
1	C	540	ARG
1	C	551	THR
1	C	556	ARG
1	C	559	ARG
1	C	614	VAL
1	C	615	GLN
1	C	630	VAL

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Mol	Chain	Res	Type
1	C	631	ARG
1	C	633	ARG
1	C	634	LEU
1	C	654	ASP
1	C	660	VAL
1	D	34	LEU
1	D	35	THR
1	D	37	ARG
1	D	39	ARG
1	D	59	VAL
1	D	62	ILE
1	D	67	LEU
1	D	68	ARG
1	D	73	LEU
1	D	93	LEU
1	D	101	ARG
1	D	103	ILE
1	D	126	LEU
1	D	133	ARG
1	D	135	ASP
1	D	137	LYS
1	D	153	VAL
1	D	173	ARG
1	D	174	MET
1	D	177	VAL
1	D	180	LYS
1	D	191	HIS
1	D	202	VAL
1	D	212	VAL
1	D	216	GLU
1	D	219	ASN
1	D	231	LEU
1	D	251	ARG
1	D	257	ARG
1	D	260	ASN
1	D	290	VAL
1	D	298	LEU
1	D	306	SER
1	D	308	LEU
1	D	347	ILE
1	D	348	GLU
1	D	349	SER

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Mol	Chain	Res	Type
1	D	350	SER
1	D	386	VAL
1	D	425	LEU
1	D	426	THR
1	D	459	SER
1	D	473	ARG
1	D	483	GLN
1	D	491	THR
1	D	497	MET
1	D	499	PHE
1	D	513	GLN
1	D	518	ARG
1	D	525	VAL
1	D	540	ARG
1	D	551	THR
1	D	558	PHE
1	D	614	VAL
1	D	633	ARG
1	D	654	ASP
1	D	660	VAL
1	D	680	ARG
1	D	681	THR
1	E	34	LEU
1	E	41	ILE
1	E	45	ILE
1	E	51	GLU
1	E	52	LEU
1	E	56	ARG
1	E	59	VAL
1	E	62	ILE
1	E	67	LEU
1	E	73	LEU
1	E	88	LYS
1	E	93	LEU
1	E	101	ARG
1	E	104	GLU
1	E	126	LEU
1	E	153	VAL
1	E	173	ARG
1	E	174	MET
1	E	177	VAL
1	E	180	LYS

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Mol	Chain	Res	Type
1	E	191	HIS
1	E	202	VAL
1	E	212	VAL
1	E	218	SER
1	E	222	ILE
1	E	231	LEU
1	E	251	ARG
1	E	260	ASN
1	E	290	VAL
1	E	292	LYS
1	E	298	LEU
1	E	302	LYS
1	E	308	LEU
1	E	347	ILE
1	E	386	VAL
1	E	425	LEU
1	E	426	THR
1	E	459	SER
1	E	460	ARG
1	E	473	ARG
1	E	483	GLN
1	E	491	THR
1	E	497	MET
1	E	499	PHE
1	E	510	GLU
1	E	518	ARG
1	E	525	VAL
1	E	540	ARG
1	E	551	THR
1	E	552	ILE
1	E	555	GLU
1	E	556	ARG
1	E	559	ARG
1	E	577	ASN
1	E	578	PHE
1	E	614	VAL
1	E	616	ASP
1	E	617	LEU
1	E	618	VAL
1	E	620	THR
1	E	622	ASN
1	E	630	VAL

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Mol	Chain	Res	Type
1	E	632	ASP
1	E	651	THR
1	E	654	ASP
1	E	661	THR
1	E	681	THR
1	F	34	LEU
1	F	37	ARG
1	F	59	VAL
1	F	62	ILE
1	F	67	LEU
1	F	68	ARG
1	F	73	LEU
1	F	88	LYS
1	F	93	LEU
1	F	94	ILE
1	F	100	MET
1	F	101	ARG
1	F	103	ILE
1	F	104	GLU
1	F	126	LEU
1	F	131	LEU
1	F	134	ARG
1	F	141	LEU
1	F	153	VAL
1	F	173	ARG
1	F	174	MET
1	F	177	VAL
1	F	180	LYS
1	F	191	HIS
1	F	202	VAL
1	F	212	VAL
1	F	218	SER
1	F	222	ILE
1	F	231	LEU
1	F	251	ARG
1	F	256	LYS
1	F	257	ARG
1	F	260	ASN
1	F	290	VAL
1	F	298	LEU
1	F	308	LEU
1	F	310	ARG

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Mol	Chain	Res	Type
1	F	347	ILE
1	F	386	VAL
1	F	425	LEU
1	F	426	THR
1	F	459	SER
1	F	483	GLN
1	F	491	THR
1	F	497	MET
1	F	499	PHE
1	F	518	ARG
1	F	525	VAL
1	F	540	ARG
1	F	551	THR
1	F	552	ILE
1	F	556	ARG
1	F	559	ARG
1	F	612	ARG
1	F	614	VAL
1	F	617	LEU
1	F	618	VAL
1	F	620	THR
1	F	622	ASN
1	F	623	ASP
1	F	628	CYS
1	F	632	ASP
1	F	654	ASP
1	F	681	THR
1	G	34	LEU
1	G	37	ARG
1	G	59	VAL
1	G	62	ILE
1	G	64	LEU
1	G	67	LEU
1	G	68	ARG
1	G	73	LEU
1	G	88	LYS
1	G	93	LEU
1	G	101	ARG
1	G	104	GLU
1	G	126	LEU
1	G	153	VAL
1	G	173	ARG

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Mol	Chain	Res	Type
1	G	174	MET
1	G	177	VAL
1	G	180	LYS
1	G	191	HIS
1	G	202	VAL
1	G	212	VAL
1	G	218	SER
1	G	220	ARG
1	G	222	ILE
1	G	231	LEU
1	G	251	ARG
1	G	260	ASN
1	G	290	VAL
1	G	297	GLU
1	G	298	LEU
1	G	308	LEU
1	G	347	ILE
1	G	386	VAL
1	G	425	LEU
1	G	426	THR
1	G	459	SER
1	G	473	ARG
1	G	483	GLN
1	G	491	THR
1	G	497	MET
1	G	499	PHE
1	G	518	ARG
1	G	525	VAL
1	G	540	ARG
1	G	551	THR
1	G	556	ARG
1	G	559	ARG
1	G	614	VAL
1	G	616	ASP
1	G	617	LEU
1	G	618	VAL
1	G	620	THR
1	G	622	ASN
1	G	632	ASP
1	G	654	ASP
1	G	680	ARG
1	G	681	THR

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Mol	Chain	Res	Type
1	H	34	LEU
1	H	59	VAL
1	H	67	LEU
1	H	73	LEU
1	H	88	LYS
1	H	93	LEU
1	H	101	ARG
1	H	104	GLU
1	H	126	LEU
1	H	153	VAL
1	H	173	ARG
1	H	174	MET
1	H	177	VAL
1	H	180	LYS
1	H	191	HIS
1	H	202	VAL
1	H	212	VAL
1	H	218	SER
1	H	222	ILE
1	H	231	LEU
1	H	253	GLN
1	H	254	ARG
1	H	260	ASN
1	H	290	VAL
1	H	298	LEU
1	H	308	LEU
1	H	347	ILE
1	H	356	ARG
1	H	386	VAL
1	H	425	LEU
1	H	426	THR
1	H	459	SER
1	H	473	ARG
1	H	483	GLN
1	H	491	THR
1	H	497	MET
1	H	499	PHE
1	H	518	ARG
1	H	525	VAL
1	H	540	ARG
1	H	551	THR
1	H	556	ARG

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Mol	Chain	Res	Type
1	H	577	ASN
1	H	579	CYS
1	H	581	CYS
1	H	614	VAL
1	H	616	ASP
1	H	617	LEU
1	H	618	VAL
1	H	620	THR
1	H	622	ASN
1	H	632	ASP
1	H	654	ASP
1	H	660	VAL
1	H	681	THR
1	I	34	LEU
1	I	35	THR
1	I	59	VAL
1	I	62	ILE
1	I	67	LEU
1	I	73	LEU
1	I	92	ARG
1	I	93	LEU
1	I	101	ARG
1	I	104	GLU
1	I	117	ILE
1	I	126	LEU
1	I	134	ARG
1	I	137	LYS
1	I	138	ASN
1	I	153	VAL
1	I	173	ARG
1	I	174	MET
1	I	177	VAL
1	I	180	LYS
1	I	191	HIS
1	I	202	VAL
1	I	212	VAL
1	I	219	ASN
1	I	220	ARG
1	I	225	LYS
1	I	231	LEU
1	I	251	ARG
1	I	260	ASN

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Mol	Chain	Res	Type
1	I	290	VAL
1	I	298	LEU
1	I	308	LEU
1	I	347	ILE
1	I	356	ARG
1	I	386	VAL
1	I	425	LEU
1	I	426	THR
1	I	459	SER
1	I	473	ARG
1	I	483	GLN
1	I	491	THR
1	I	497	MET
1	I	499	PHE
1	I	518	ARG
1	I	525	VAL
1	I	540	ARG
1	I	551	THR
1	I	556	ARG
1	I	559	ARG
1	I	609	GLU
1	I	614	VAL
1	I	616	ASP
1	I	617	LEU
1	I	618	VAL
1	I	620	THR
1	I	622	ASN
1	I	631	ARG
1	I	634	LEU
1	I	647	ARG
1	I	648	LEU
1	I	654	ASP
1	I	660	VAL
1	I	681	THR
1	J	34	LEU
1	J	51	GLU
1	J	52	LEU
1	J	59	VAL
1	J	62	ILE
1	J	67	LEU
1	J	73	LEU
1	J	93	LEU

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Mol	Chain	Res	Type
1	J	101	ARG
1	J	104	GLU
1	J	126	LEU
1	J	153	VAL
1	J	172	MET
1	J	173	ARG
1	J	177	VAL
1	J	180	LYS
1	J	191	HIS
1	J	202	VAL
1	J	212	VAL
1	J	218	SER
1	J	222	ILE
1	J	231	LEU
1	J	251	ARG
1	J	260	ASN
1	J	290	VAL
1	J	298	LEU
1	J	308	LEU
1	J	347	ILE
1	J	349	SER
1	J	386	VAL
1	J	425	LEU
1	J	426	THR
1	J	428	GLU
1	J	460	ARG
1	J	483	GLN
1	J	491	THR
1	J	497	MET
1	J	499	PHE
1	J	518	ARG
1	J	525	VAL
1	J	540	ARG
1	J	551	THR
1	J	556	ARG
1	J	559	ARG
1	J	579	CYS
1	J	609	GLU
1	J	614	VAL
1	J	616	ASP
1	J	617	LEU
1	J	618	VAL

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Mol	Chain	Res	Type
1	J	620	THR
1	J	622	ASN
1	J	632	ASP
1	J	654	ASP
1	J	660	VAL
1	J	680	ARG
1	J	681	THR
1	K	34	LEU
1	K	59	VAL
1	K	62	ILE
1	K	67	LEU
1	K	73	LEU
1	K	88	LYS
1	K	93	LEU
1	K	101	ARG
1	K	104	GLU
1	K	126	LEU
1	K	153	VAL
1	K	173	ARG
1	K	174	MET
1	K	177	VAL
1	K	180	LYS
1	K	191	HIS
1	K	202	VAL
1	K	212	VAL
1	K	218	SER
1	K	222	ILE
1	K	231	LEU
1	K	254	ARG
1	K	257	ARG
1	K	260	ASN
1	K	290	VAL
1	K	298	LEU
1	K	308	LEU
1	K	347	ILE
1	K	349	SER
1	K	386	VAL
1	K	425	LEU
1	K	426	THR
1	K	459	SER
1	K	483	GLN
1	K	491	THR

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Mol	Chain	Res	Type
1	K	497	MET
1	K	499	PHE
1	K	518	ARG
1	K	525	VAL
1	K	540	ARG
1	K	551	THR
1	K	556	ARG
1	K	559	ARG
1	K	609	GLU
1	K	616	ASP
1	K	617	LEU
1	K	618	VAL
1	K	621	CYS
1	K	622	ASN
1	K	632	ASP
1	K	654	ASP
1	K	660	VAL
1	K	681	THR
1	L	34	LEU
1	L	59	VAL
1	L	62	ILE
1	L	67	LEU
1	L	68	ARG
1	L	73	LEU
1	L	81	LEU
1	L	89	ILE
1	L	92	ARG
1	L	93	LEU
1	L	98	MET
1	L	101	ARG
1	L	104	GLU
1	L	126	LEU
1	L	153	VAL
1	L	173	ARG
1	L	174	MET
1	L	177	VAL
1	L	180	LYS
1	L	191	HIS
1	L	202	VAL
1	L	212	VAL
1	L	218	SER
1	L	219	ASN

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Mol	Chain	Res	Type
1	L	220	ARG
1	L	222	ILE
1	L	231	LEU
1	L	251	ARG
1	L	253	GLN
1	L	257	ARG
1	L	260	ASN
1	L	290	VAL
1	L	298	LEU
1	L	308	LEU
1	L	347	ILE
1	L	349	SER
1	L	386	VAL
1	L	425	LEU
1	L	426	THR
1	L	459	SER
1	L	473	ARG
1	L	483	GLN
1	L	491	THR
1	L	497	MET
1	L	499	PHE
1	L	518	ARG
1	L	525	VAL
1	L	540	ARG
1	L	551	THR
1	L	556	ARG
1	L	559	ARG
1	L	614	VAL
1	L	616	ASP
1	L	617	LEU
1	L	618	VAL
1	L	620	THR
1	L	622	ASN
1	L	632	ASP
1	L	654	ASP
1	L	660	VAL
1	L	681	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN

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Mol	Chain	Res	Type
1	A	160	GLN
1	A	203	ASN
1	A	205	HIS
1	A	219	ASN
1	A	259	ASN
1	A	295	ASN
1	A	303	GLN
1	A	357	GLN
1	A	378	HIS
1	A	483	GLN
1	A	487	GLN
1	A	539	ASN
1	A	615	GLN
1	A	667	GLN
1	A	673	HIS
1	B	46	GLN
1	B	160	GLN
1	B	203	ASN
1	B	219	ASN
1	B	303	GLN
1	B	378	HIS
1	B	615	GLN
1	B	667	GLN
1	C	46	GLN
1	C	86	HIS
1	C	138	ASN
1	C	203	ASN
1	C	253	GLN
1	C	295	ASN
1	C	303	GLN
1	C	330	ASN
1	C	378	HIS
1	C	483	GLN
1	C	615	GLN
1	C	667	GLN
1	C	673	HIS
1	D	46	GLN
1	D	138	ASN
1	D	203	ASN
1	D	253	GLN
1	D	259	ASN
1	D	303	GLN

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Mol	Chain	Res	Type
1	D	378	HIS
1	D	483	GLN
1	D	615	GLN
1	D	667	GLN
1	D	673	HIS
1	E	47	ASN
1	E	203	ASN
1	E	208	HIS
1	E	259	ASN
1	E	295	ASN
1	E	303	GLN
1	E	330	ASN
1	E	378	HIS
1	E	469	ASN
1	E	615	GLN
1	E	622	ASN
1	E	667	GLN
1	E	673	HIS
1	F	46	GLN
1	F	203	ASN
1	F	303	GLN
1	F	330	ASN
1	F	378	HIS
1	F	667	GLN
1	F	673	HIS
1	G	46	GLN
1	G	203	ASN
1	G	259	ASN
1	G	303	GLN
1	G	378	HIS
1	G	615	GLN
1	G	622	ASN
1	G	667	GLN
1	G	673	HIS
1	H	46	GLN
1	H	203	ASN
1	H	259	ASN
1	H	295	ASN
1	H	303	GLN
1	H	378	HIS
1	H	483	GLN
1	H	577	ASN

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Mol	Chain	Res	Type
1	H	615	GLN
1	H	622	ASN
1	H	667	GLN
1	H	673	HIS
1	I	46	GLN
1	I	76	GLN
1	I	203	ASN
1	I	259	ASN
1	I	303	GLN
1	I	622	ASN
1	I	667	GLN
1	I	673	HIS
1	J	203	ASN
1	J	259	ASN
1	J	303	GLN
1	J	378	HIS
1	J	508	ASN
1	J	615	GLN
1	J	622	ASN
1	J	667	GLN
1	J	673	HIS
1	K	46	GLN
1	K	76	GLN
1	K	203	ASN
1	K	253	GLN
1	K	295	ASN
1	K	303	GLN
1	K	622	ASN
1	K	667	GLN
1	K	673	HIS
1	L	203	ASN
1	L	205	HIS
1	L	259	ASN
1	L	295	ASN
1	L	303	GLN
1	L	378	HIS
1	L	479	HIS
1	L	508	ASN
1	L	615	GLN
1	L	622	ASN
1	L	667	GLN
1	L	673	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 24 are monoatomic - leaving 7 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	EDO	D	704	-	3,3,3	0.24	0	2,2,2	0.40	0
3	EDO	D	703	-	3,3,3	0.59	0	2,2,2	0.50	0
3	EDO	A	704	-	3,3,3	0.34	0	2,2,2	0.47	0
3	EDO	H	703	-	3,3,3	0.18	0	2,2,2	0.25	0
3	EDO	A	705	-	3,3,3	0.20	0	2,2,2	0.33	0
3	EDO	F	703	-	3,3,3	0.08	0	2,2,2	0.09	0
3	EDO	A	703	-	3,3,3	0.24	0	2,2,2	0.33	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	EDO	D	704	-	-	0/1/1/1	-
3	EDO	D	703	-	-	1/1/1/1	-
3	EDO	A	704	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	H	703	-	-	1/1/1/1	-
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	F	703	-	-	1/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	704	EDO	O1-C1-C2-O2
3	H	703	EDO	O1-C1-C2-O2
3	D	703	EDO	O1-C1-C2-O2
3	F	703	EDO	O1-C1-C2-O2

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	651/681 (95%)	-1.58	0 100 100	26, 55, 102, 177	0
1	B	645/681 (94%)	-1.55	0 100 100	27, 62, 105, 177	0
1	C	648/681 (95%)	-1.55	0 100 100	21, 60, 107, 194	0
1	D	650/681 (95%)	-1.56	0 100 100	23, 59, 105, 181	0
1	E	661/681 (97%)	-1.56	0 100 100	28, 62, 113, 160	0
1	F	657/681 (96%)	-1.53	0 100 100	29, 64, 115, 177	0
1	G	659/681 (96%)	-1.58	0 100 100	27, 59, 109, 192	0
1	H	661/681 (97%)	-1.58	0 100 100	28, 60, 117, 214	0
1	I	660/681 (96%)	-1.52	0 100 100	28, 66, 127, 189	0
1	J	659/681 (96%)	-1.54	0 100 100	26, 67, 124, 219	0
1	K	660/681 (96%)	-1.53	0 100 100	32, 69, 128, 181	0
1	L	659/681 (96%)	-1.49	0 100 100	26, 70, 127, 198	0
All	All	7870/8172 (96%)	-1.55	0 100 100	21, 63, 116, 219	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

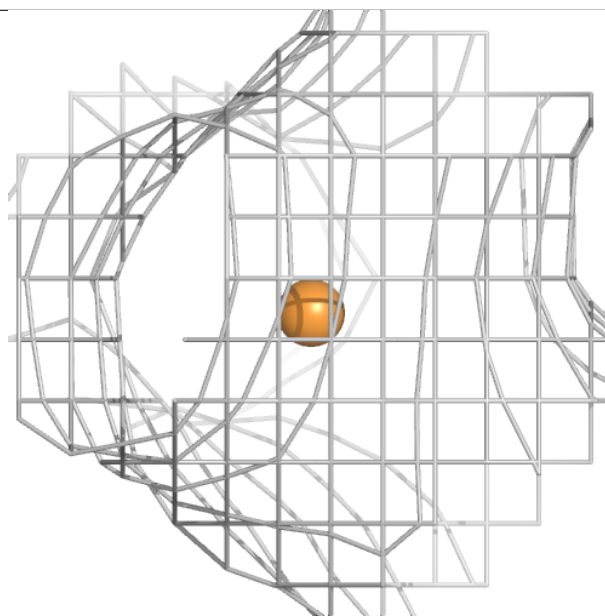
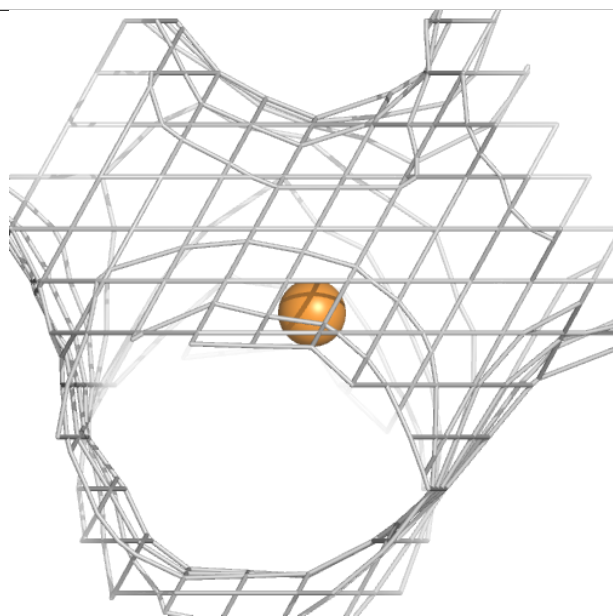
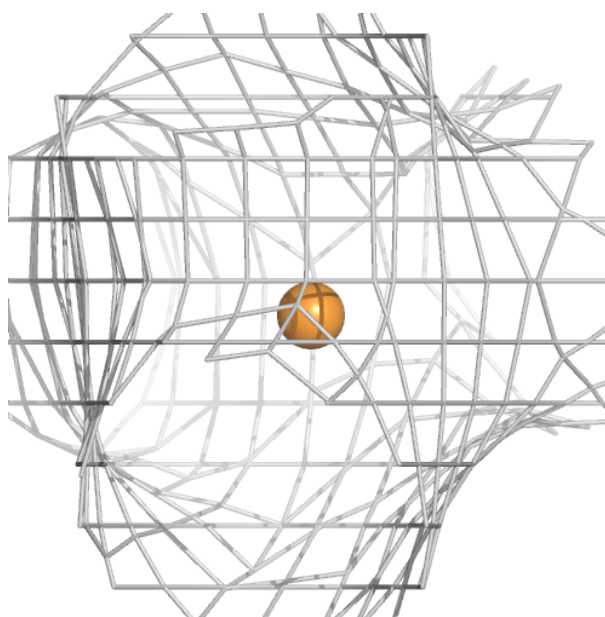
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	F	703	4/4	0.95	0.09	57,61,61,62	0
3	EDO	D	704	4/4	0.97	0.06	46,47,48,49	0
3	EDO	A	705	4/4	0.98	0.04	56,58,60,61	0
3	EDO	D	703	4/4	0.98	0.05	21,24,25,25	0
3	EDO	A	703	4/4	0.99	0.04	23,25,27,28	0
3	EDO	A	704	4/4	0.99	0.04	33,36,39,39	0
3	EDO	H	703	4/4	0.99	0.07	50,51,51,51	0
2	CU	D	702	1/1	1.00	0.02	65,65,65,65	0
2	CU	E	701	1/1	1.00	0.03	81,81,81,81	0
2	CU	E	702	1/1	1.00	0.03	56,56,56,56	0
2	CU	F	701	1/1	1.00	0.02	62,62,62,62	0
2	CU	F	702	1/1	1.00	0.01	57,57,57,57	0
2	CU	G	701	1/1	1.00	0.01	56,56,56,56	0
2	CU	G	702	1/1	1.00	0.02	66,66,66,66	0
2	CU	H	701	1/1	1.00	0.01	52,52,52,52	0
2	CU	H	702	1/1	1.00	0.01	47,47,47,47	0
2	CU	I	701	1/1	1.00	0.02	60,60,60,60	0
2	CU	I	702	1/1	1.00	0.02	73,73,73,73	0
2	CU	J	701	1/1	1.00	0.01	73,73,73,73	0
2	CU	J	702	1/1	1.00	0.01	66,66,66,66	0
2	CU	K	701	1/1	1.00	0.01	75,75,75,75	0
2	CU	K	702	1/1	1.00	0.01	57,57,57,57	0
2	CU	L	701	1/1	1.00	0.02	66,66,66,66	0
2	CU	L	702	1/1	1.00	0.01	53,53,53,53	0
2	CU	A	701	1/1	1.00	0.03	55,55,55,55	0
2	CU	A	702	1/1	1.00	0.03	61,61,61,61	0
2	CU	B	701	1/1	1.00	0.01	64,64,64,64	0
2	CU	B	702	1/1	1.00	0.03	56,56,56,56	0
2	CU	C	701	1/1	1.00	0.02	59,59,59,59	0
2	CU	C	702	1/1	1.00	0.03	46,46,46,46	0
2	CU	D	701	1/1	1.00	0.01	44,44,44,44	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.

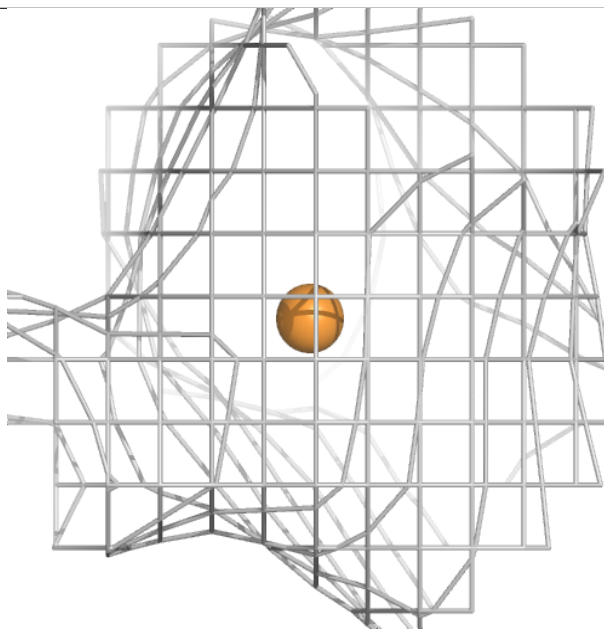
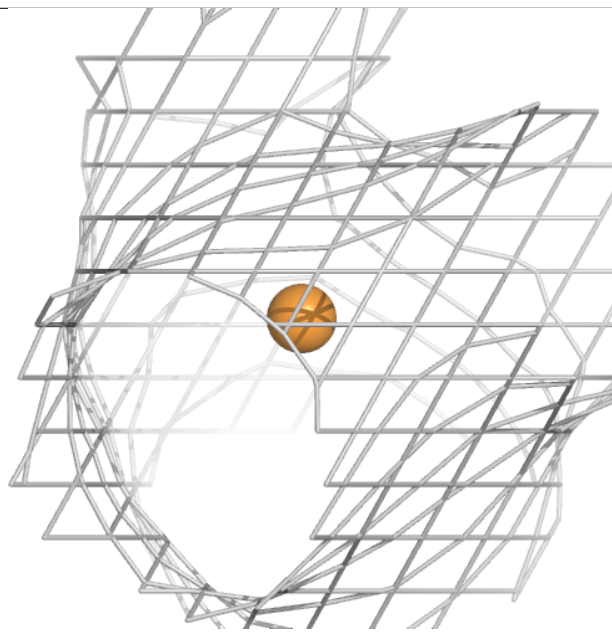
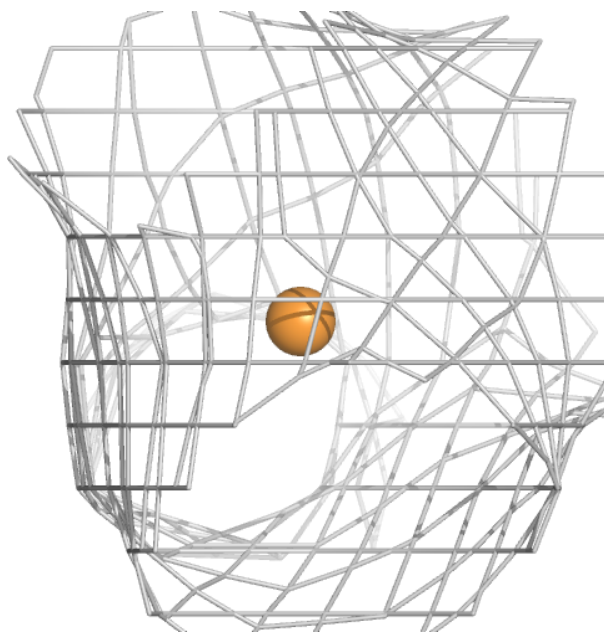
Electron density around CU D 702:

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and green (positive)



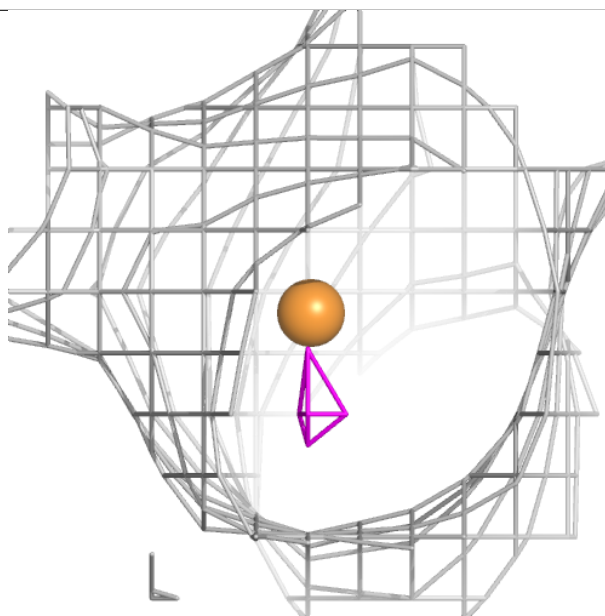
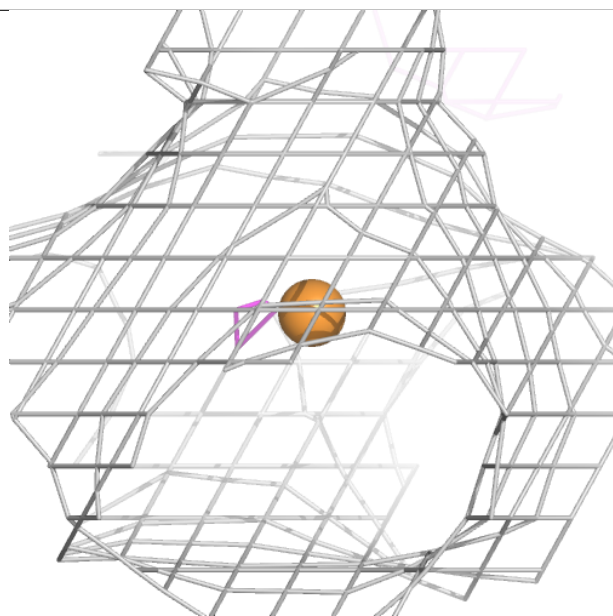
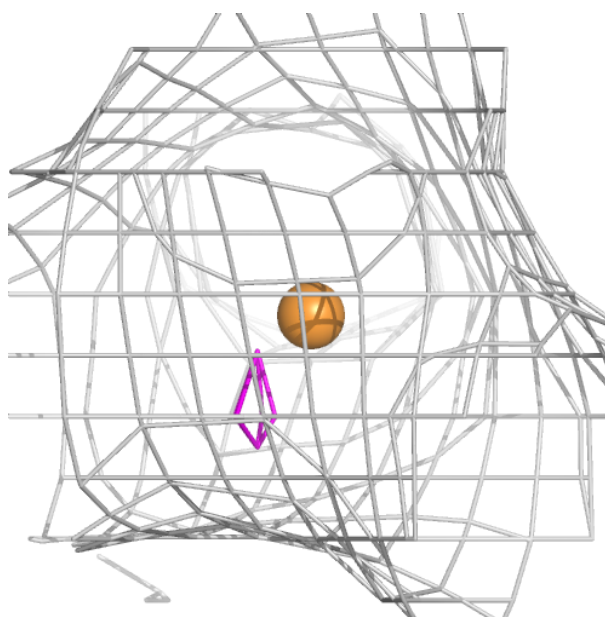
Electron density around CU E 701:

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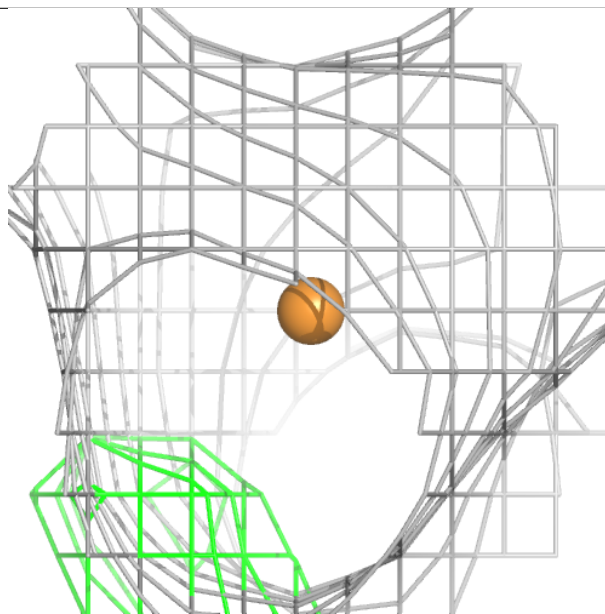
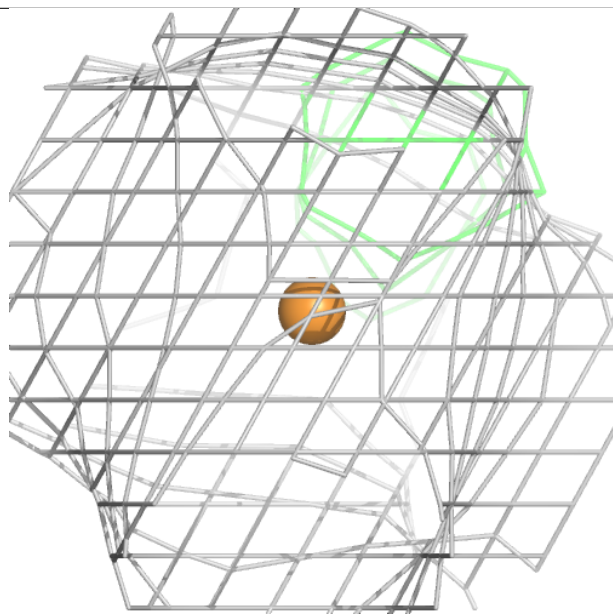
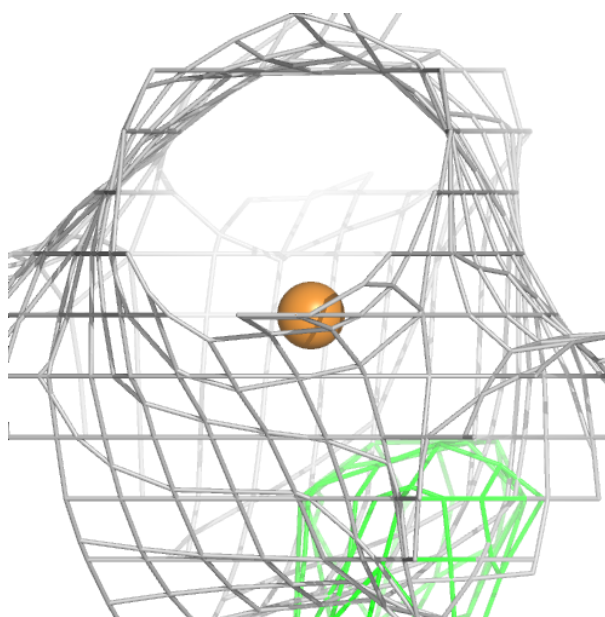
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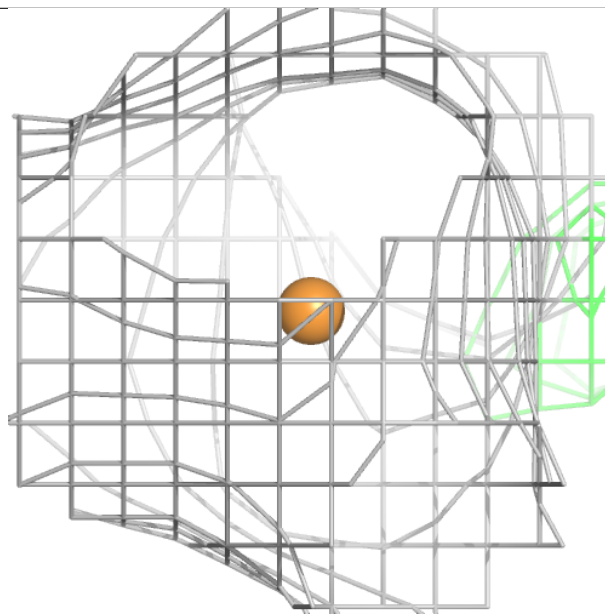
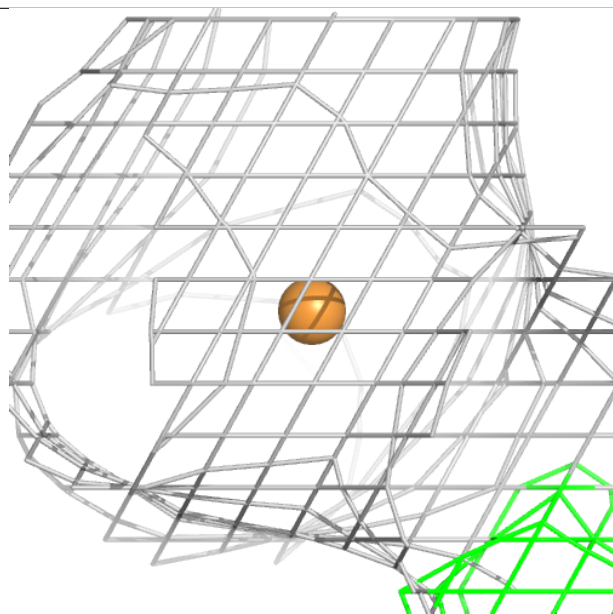
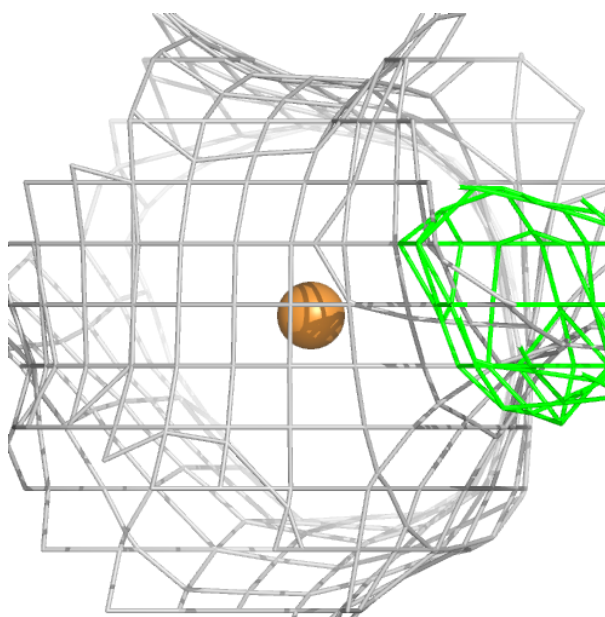
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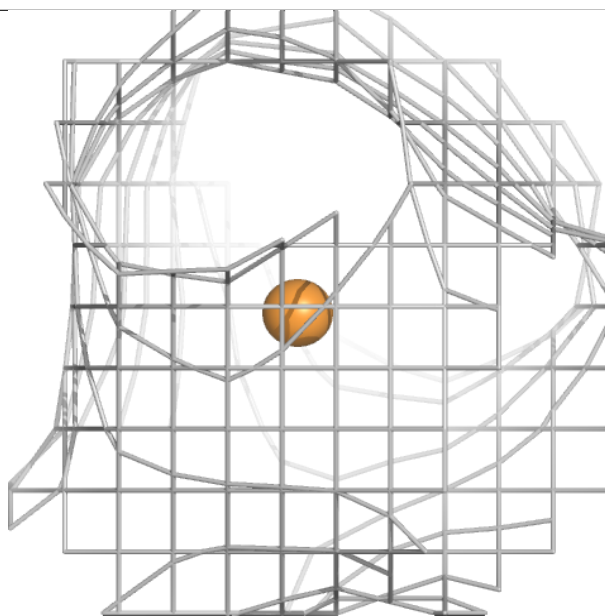
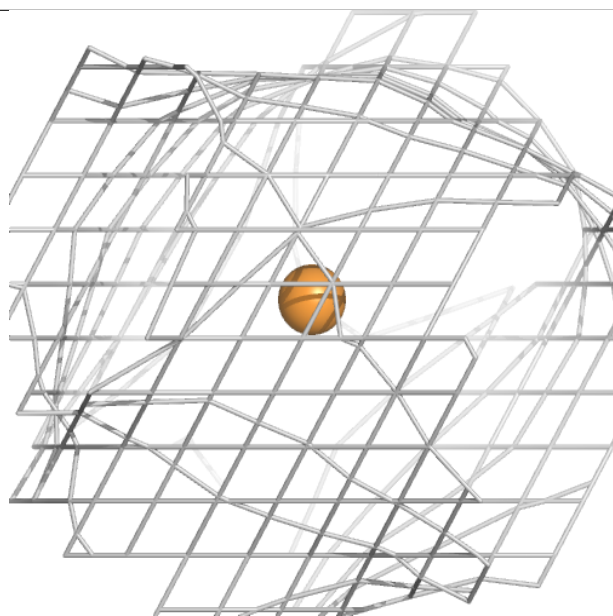
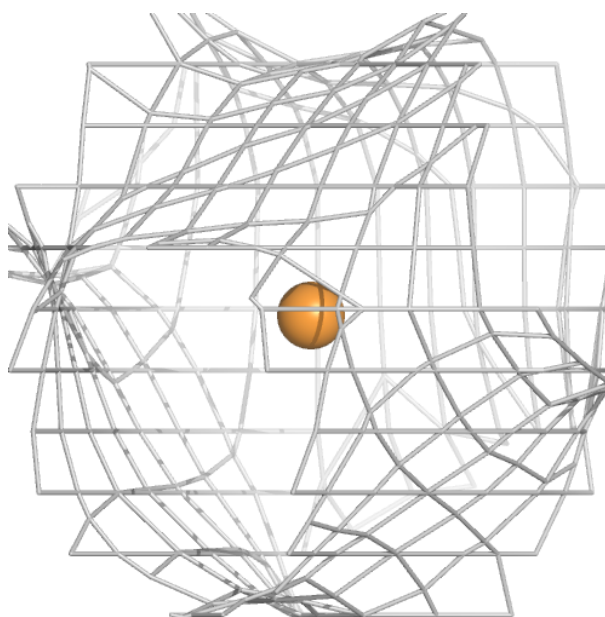
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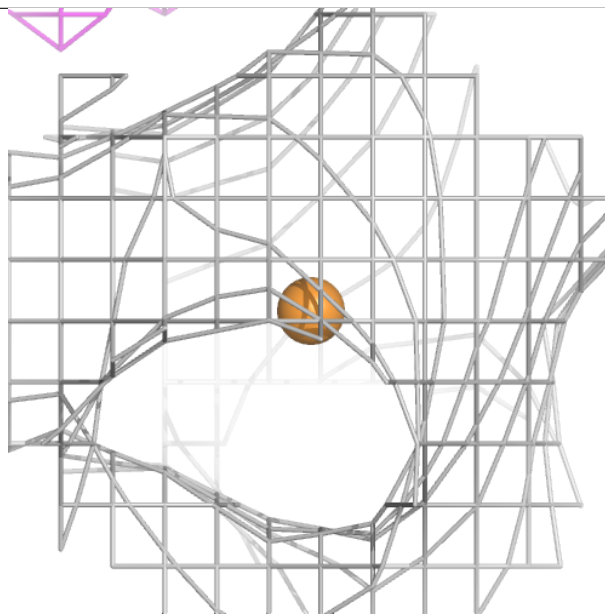
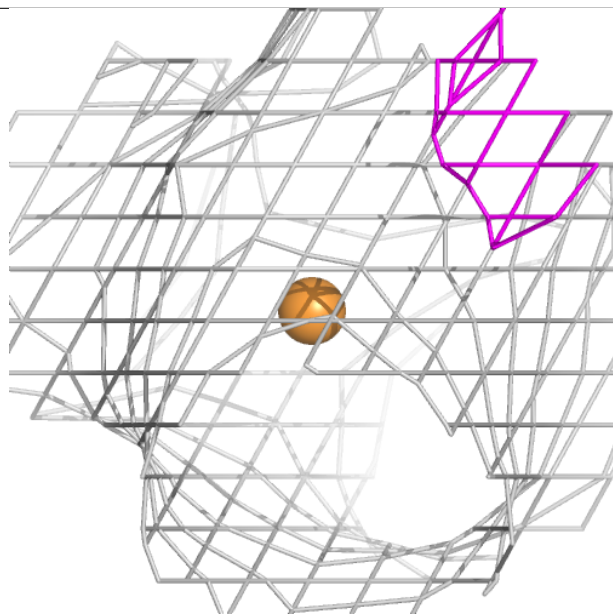
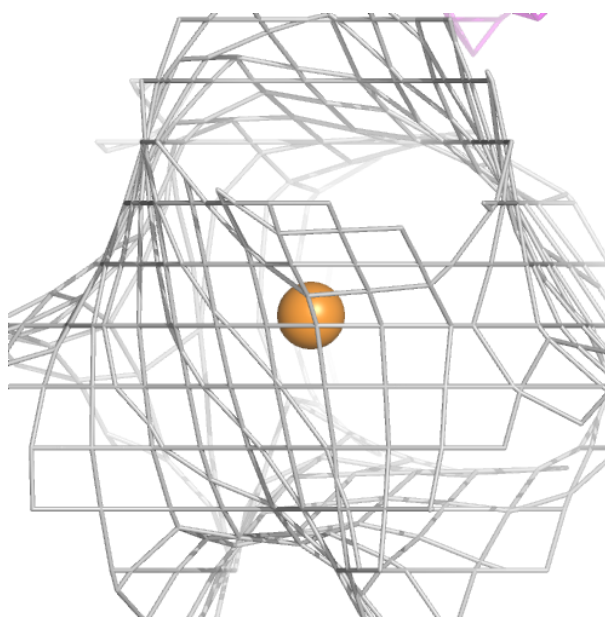
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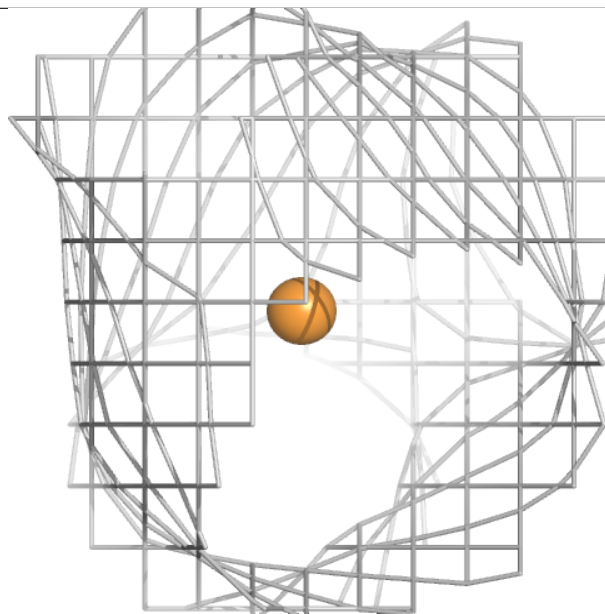
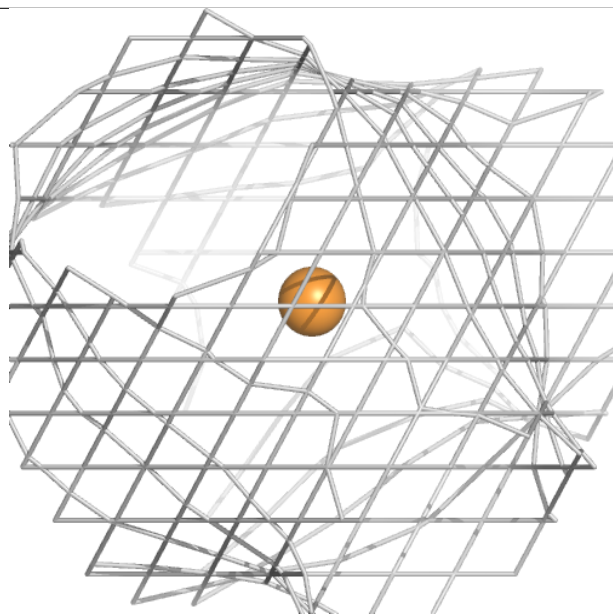
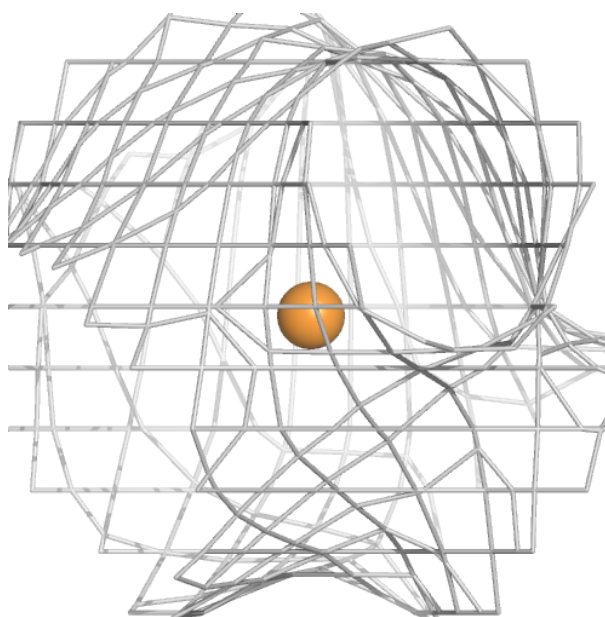
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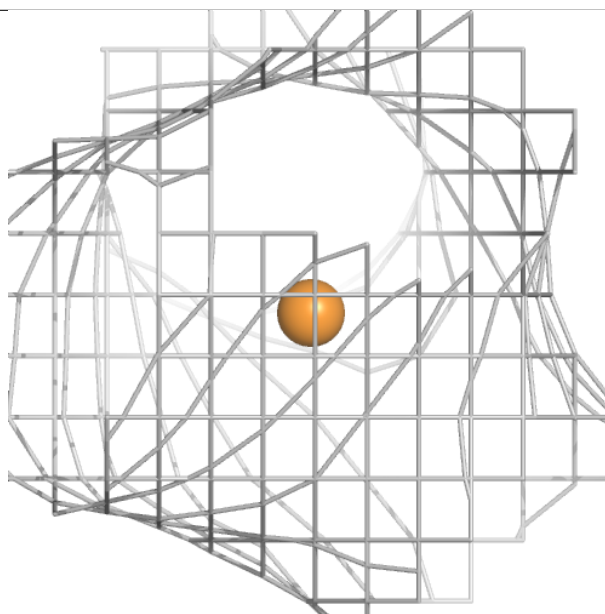
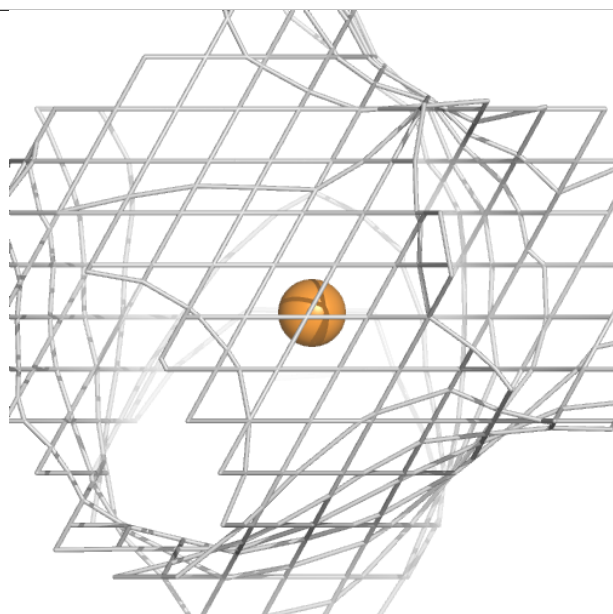
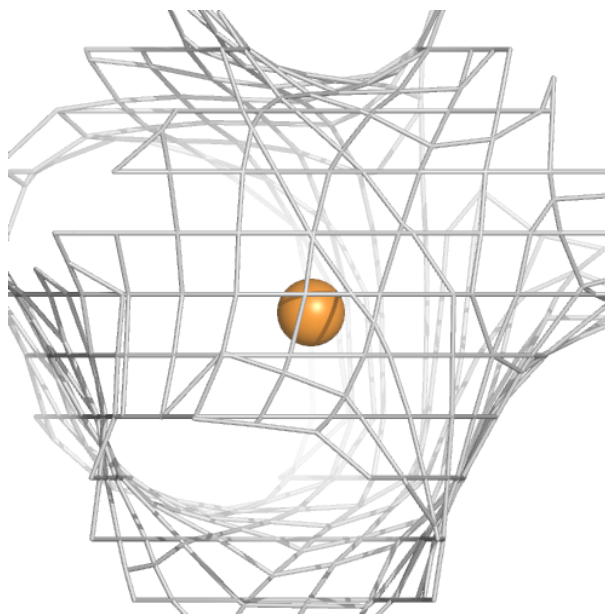
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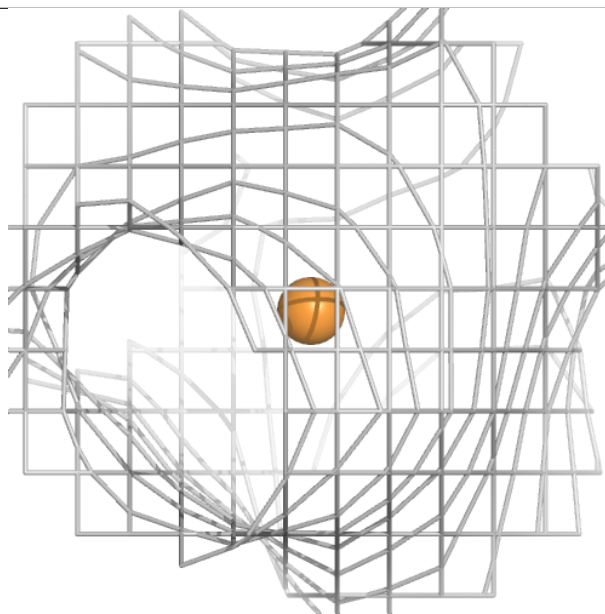
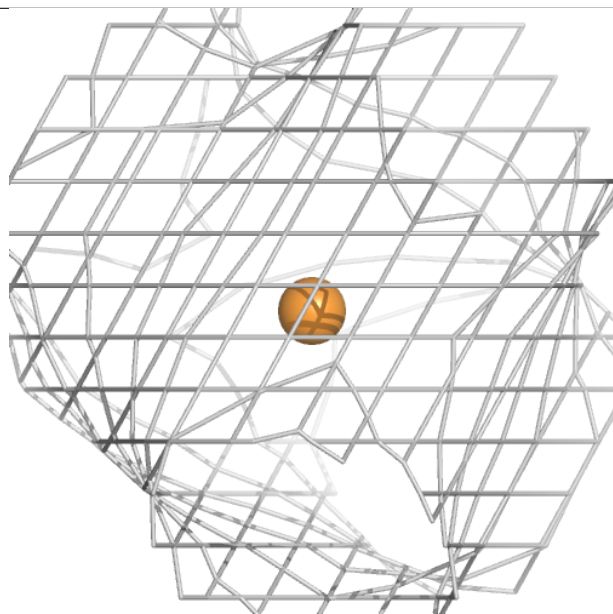
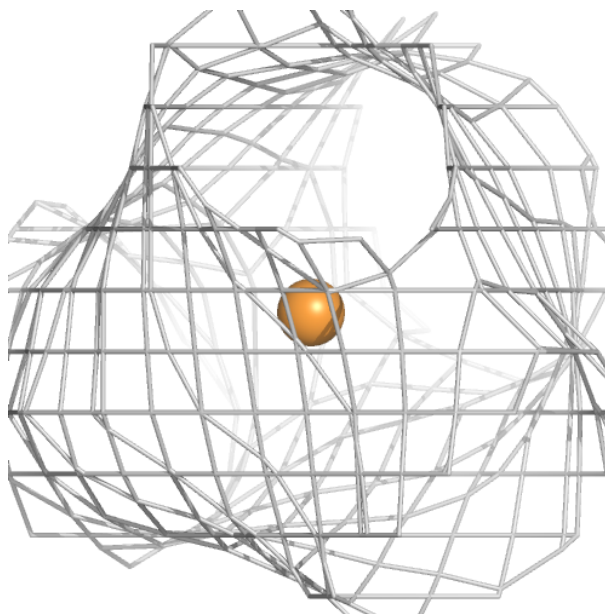
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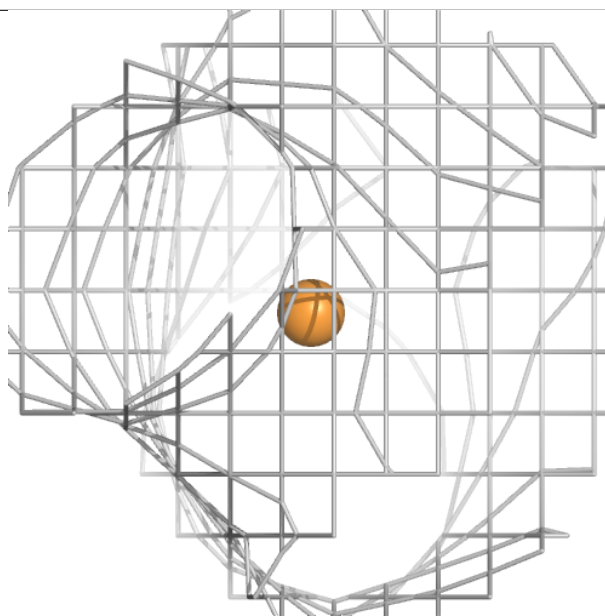
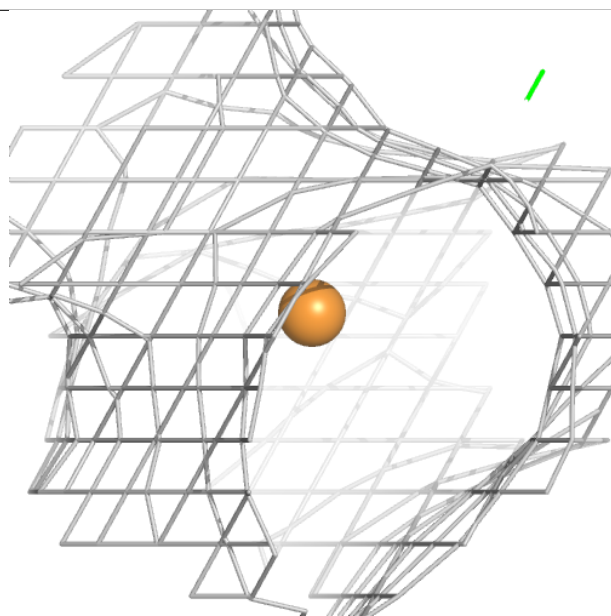
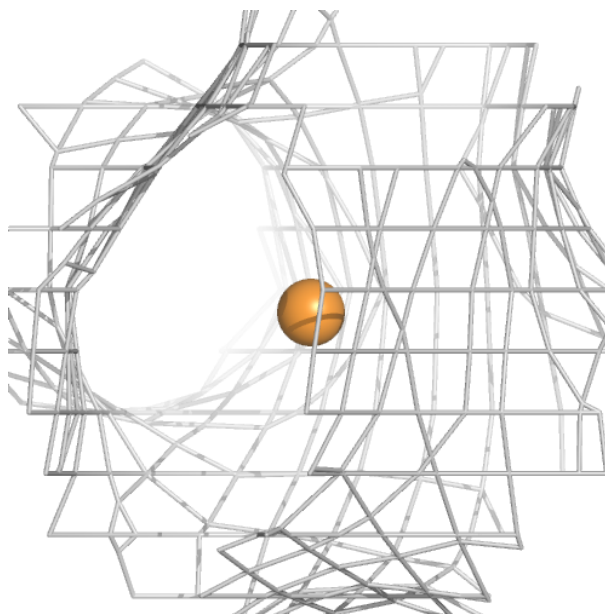
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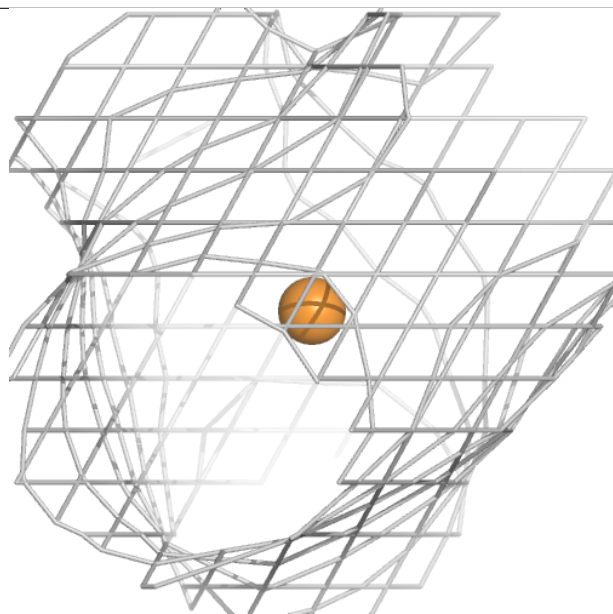
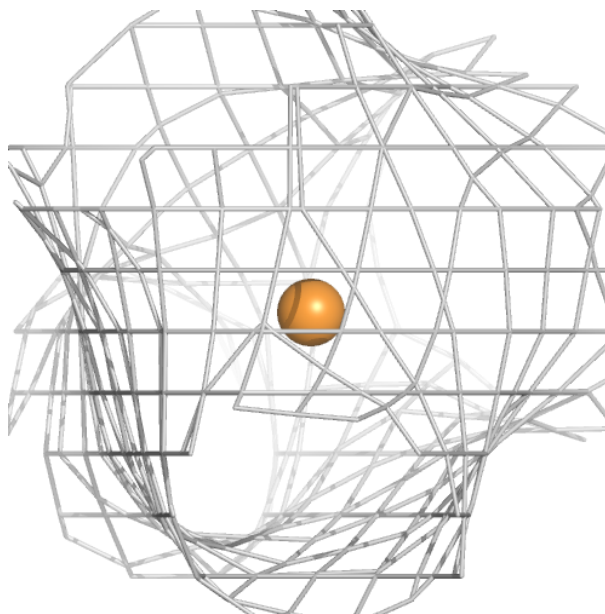
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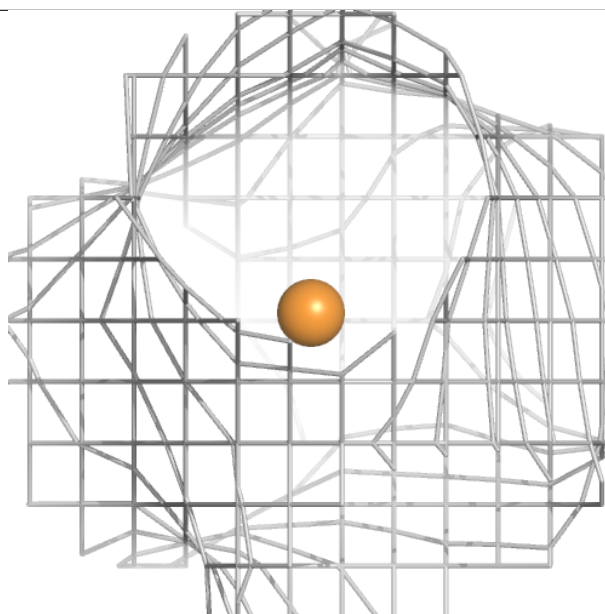
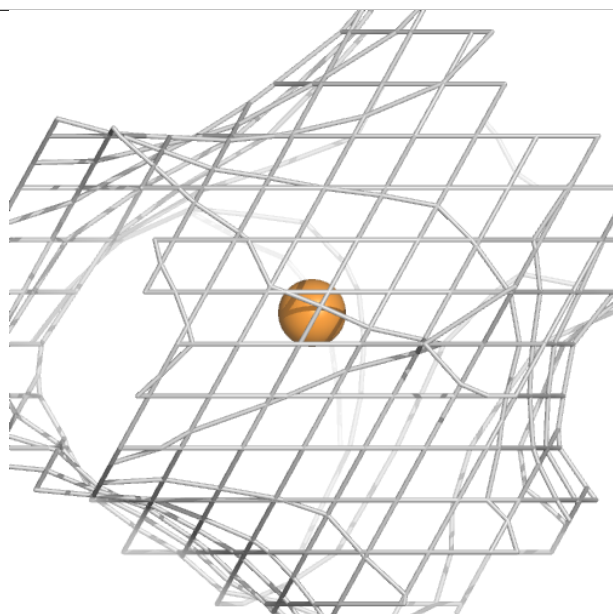
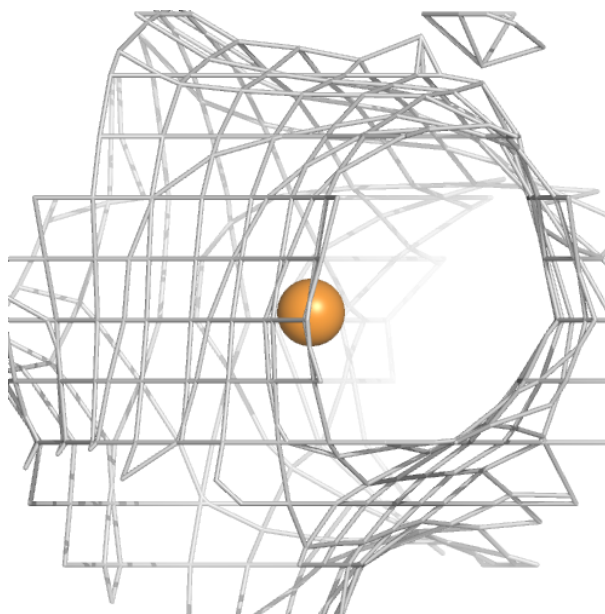
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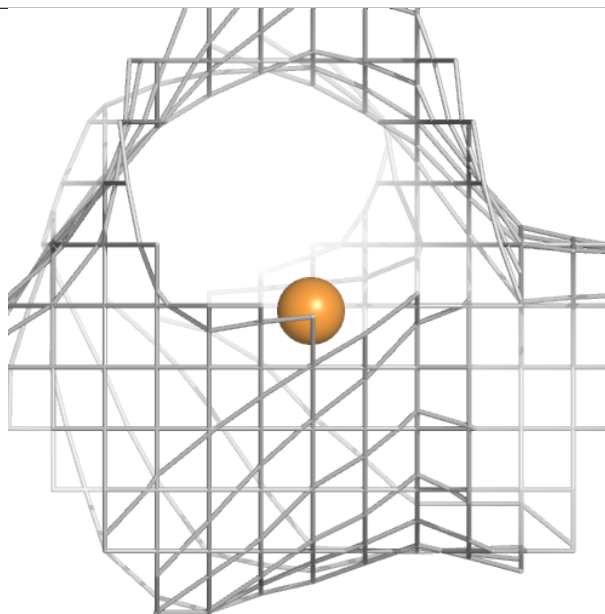
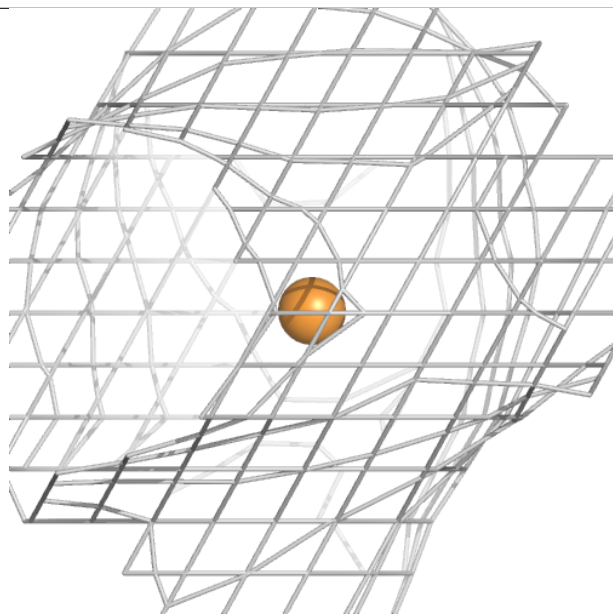
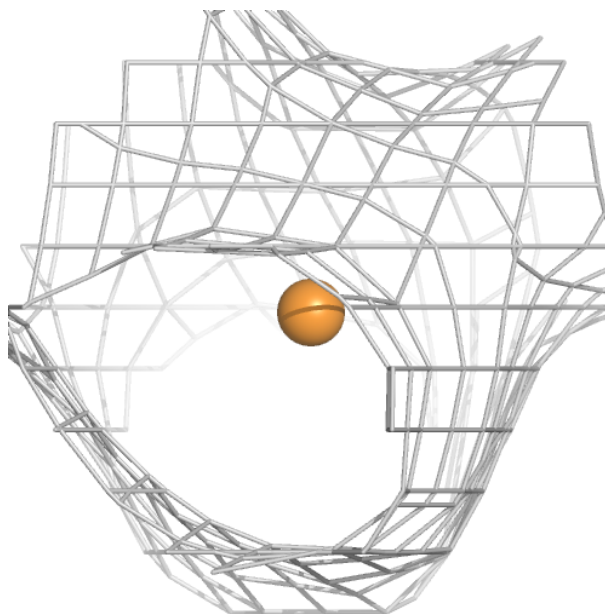
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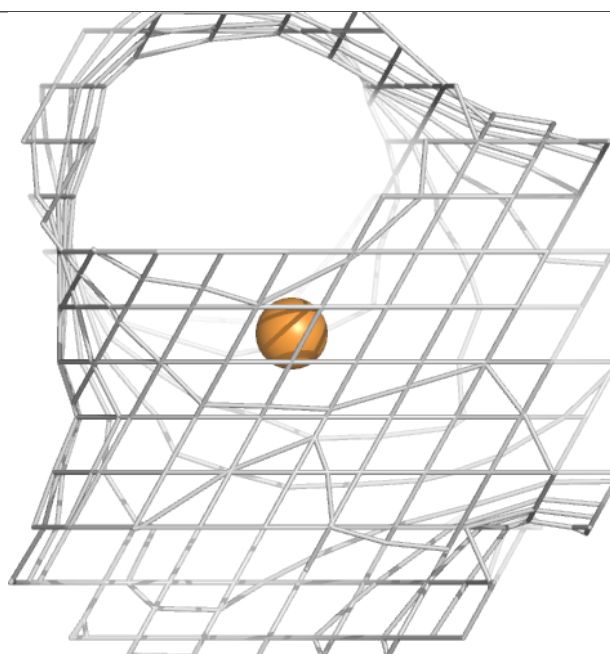
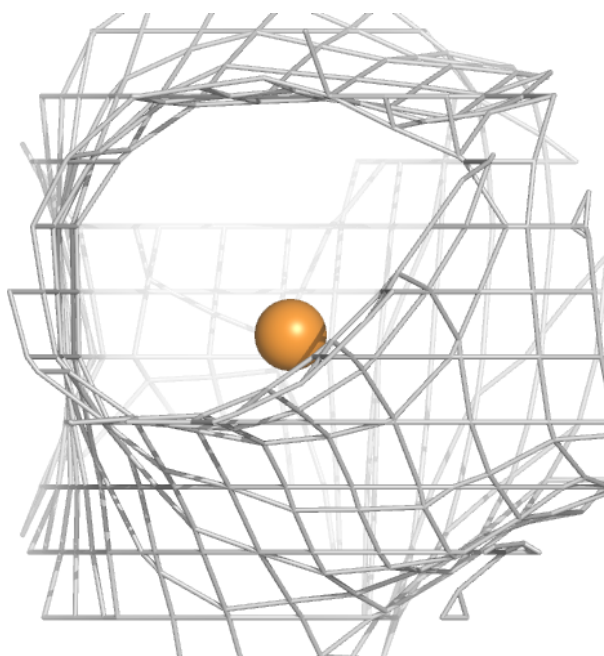
Electron density around CU K 701:

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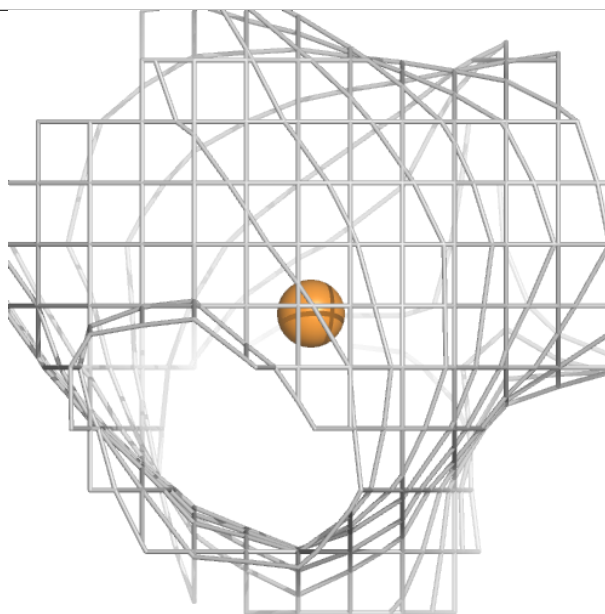
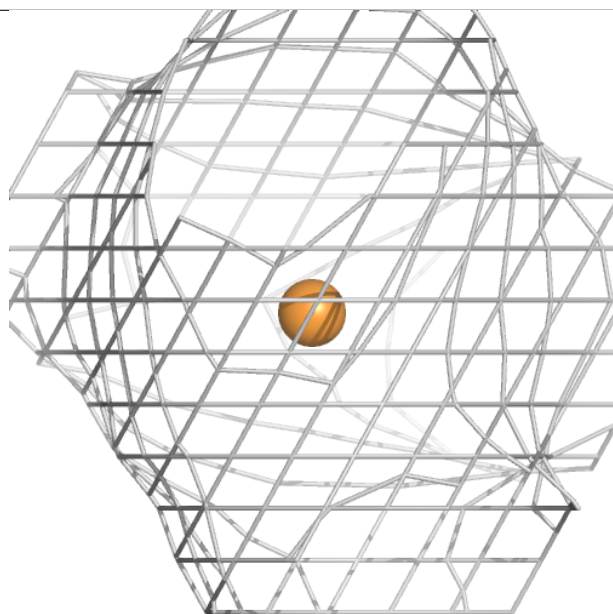
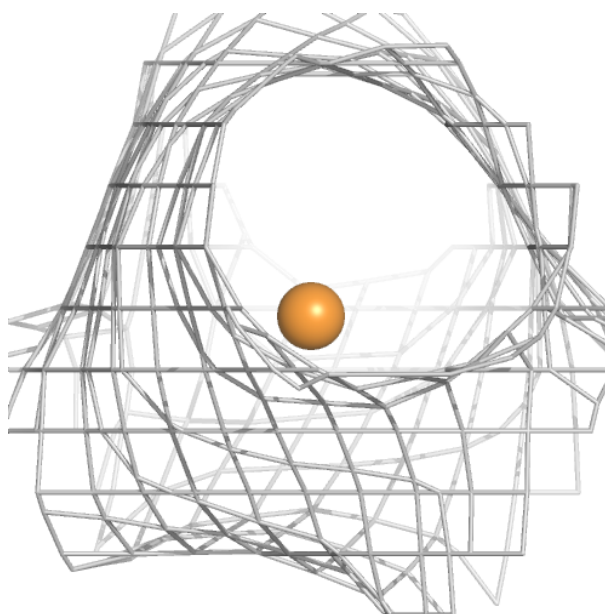
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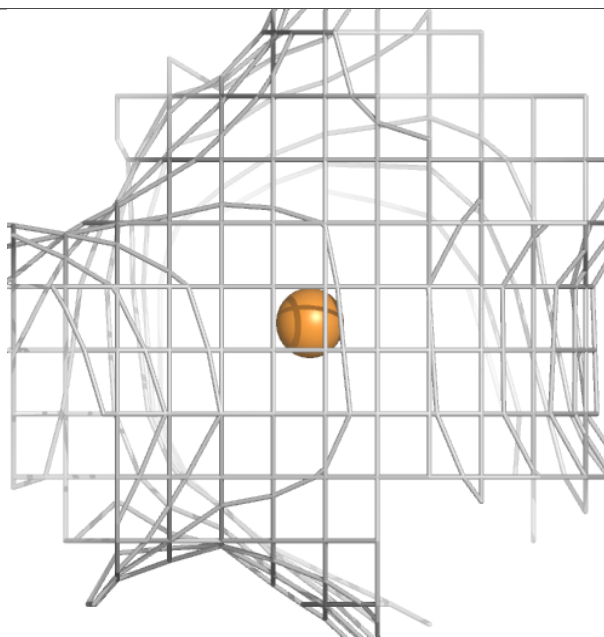
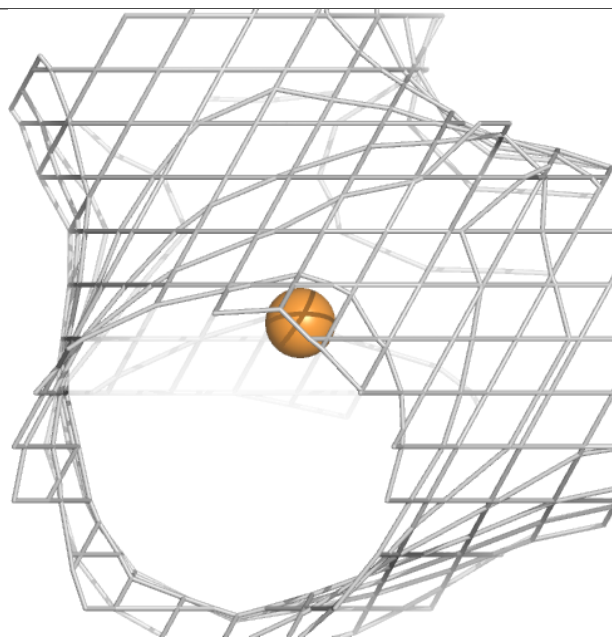
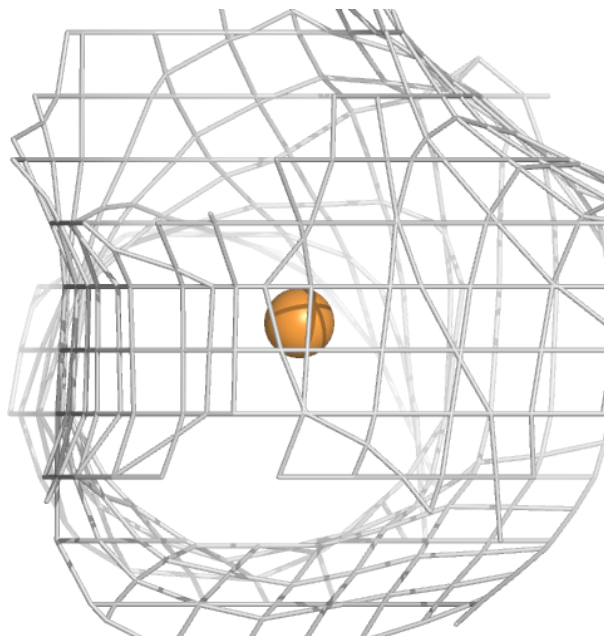
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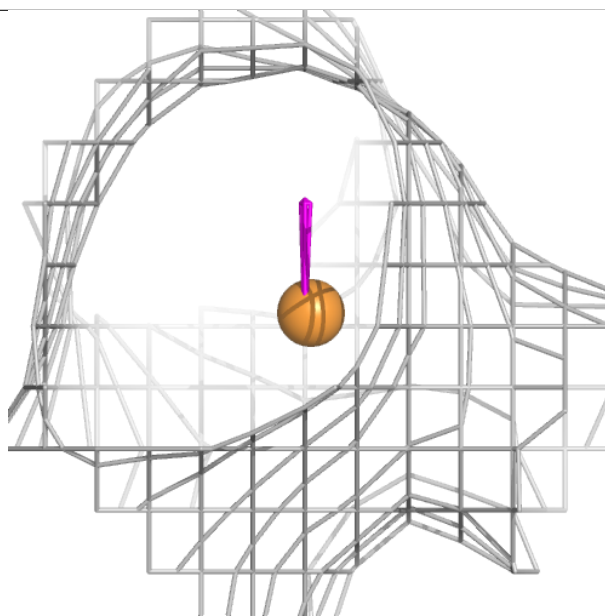
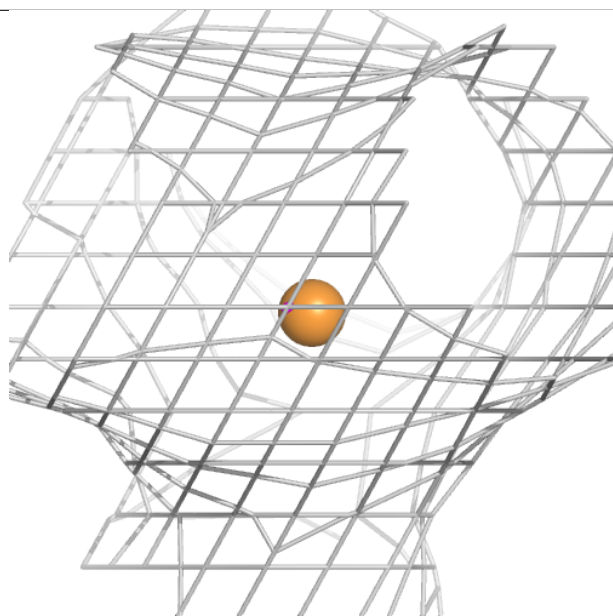
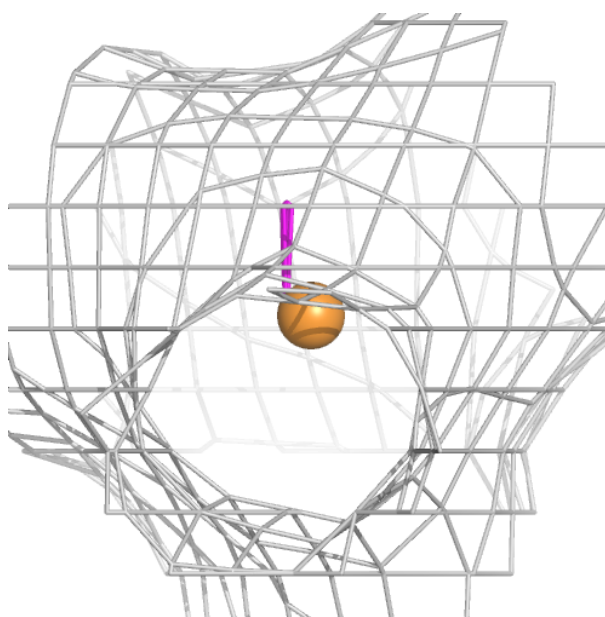
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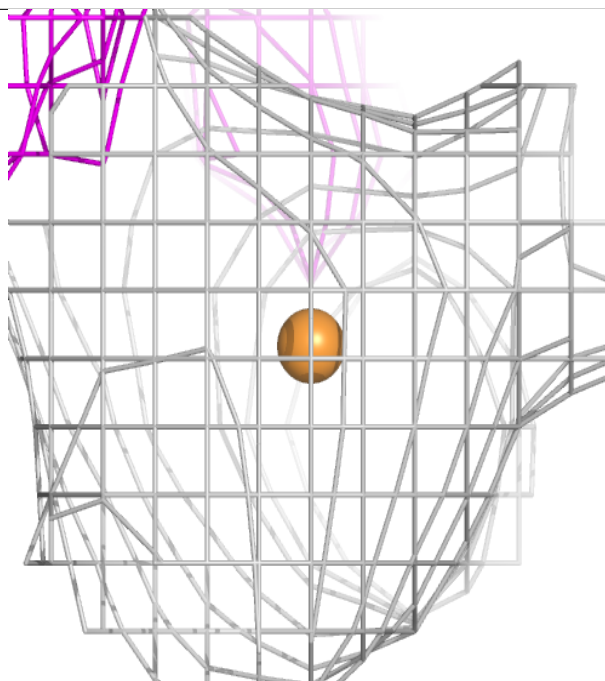
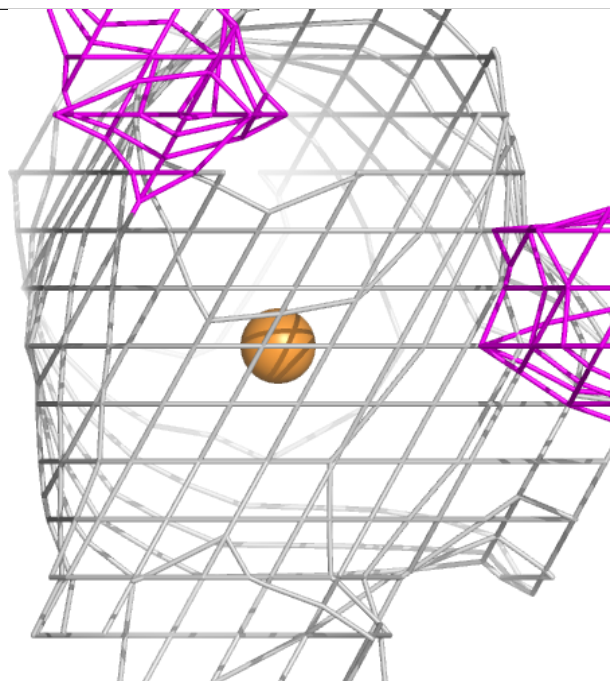
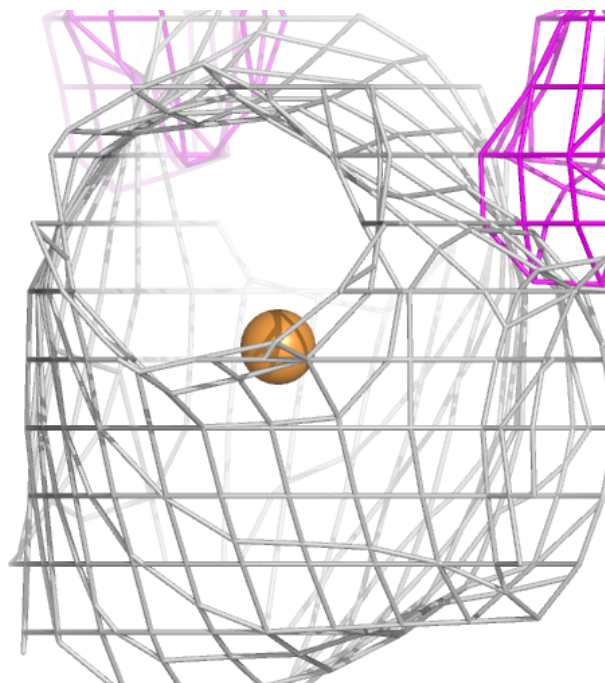
Electron density around CU A 701:

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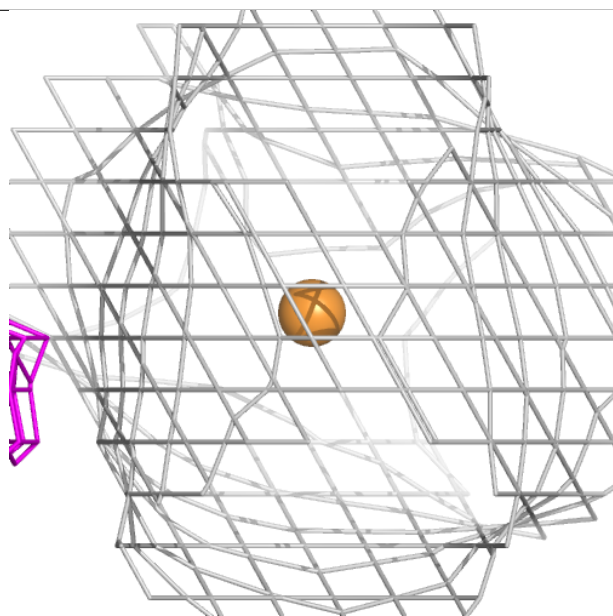
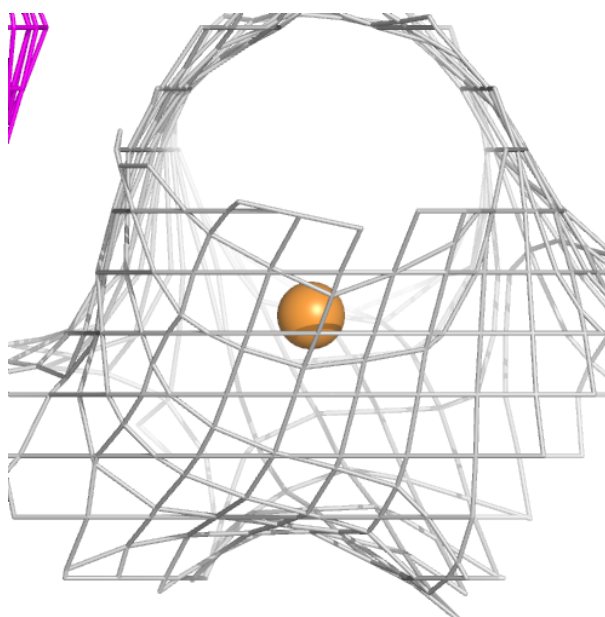
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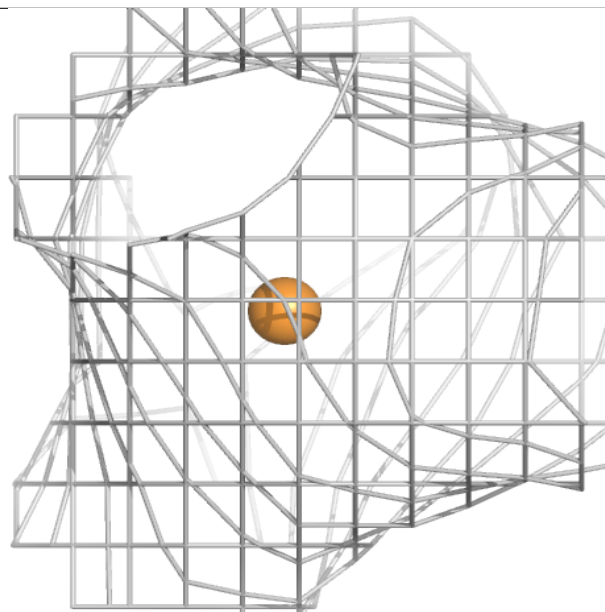
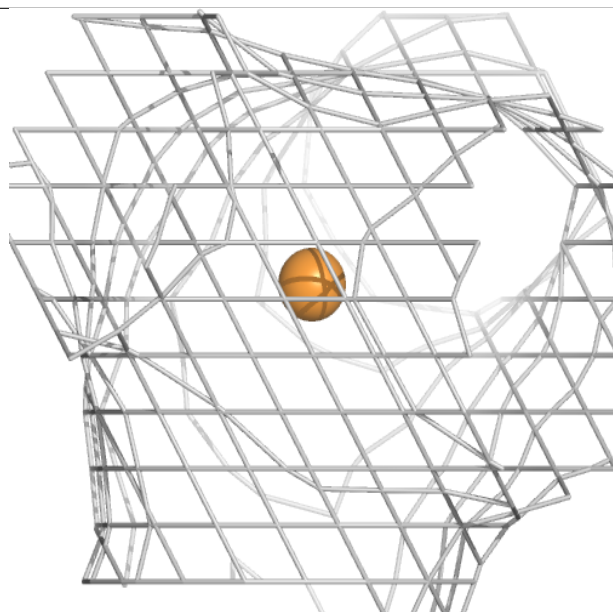
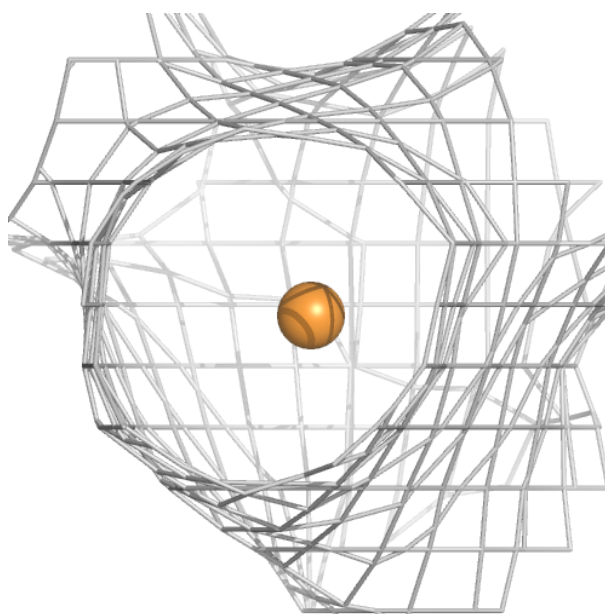
Electron density around CU B 701:

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and green (positive)



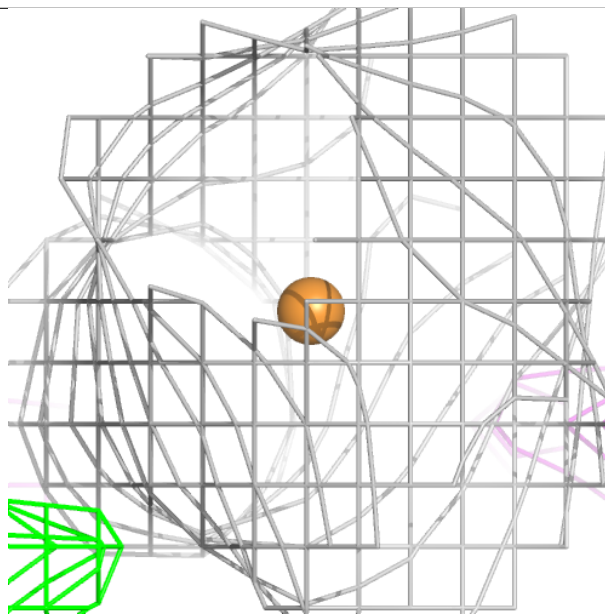
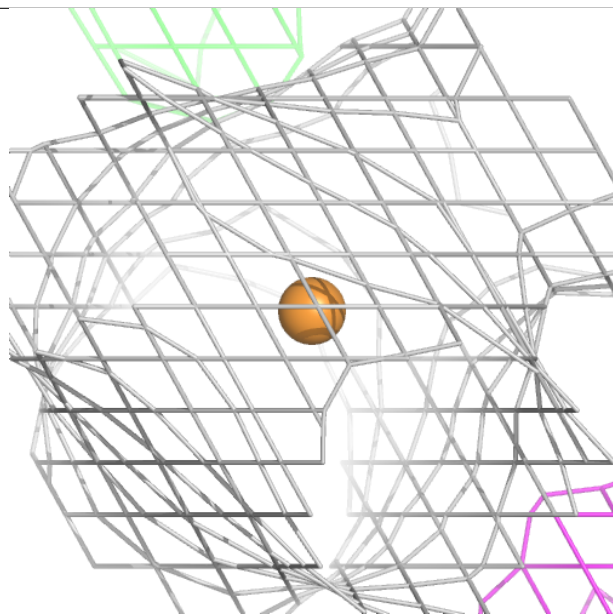
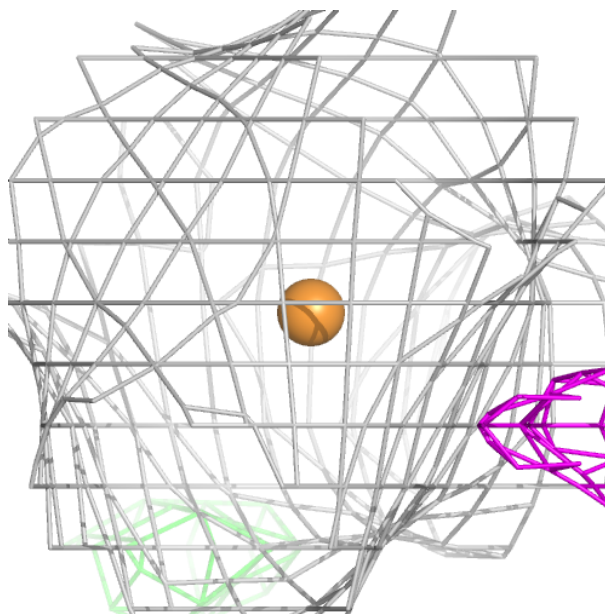
Electron density around CU B 702:

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



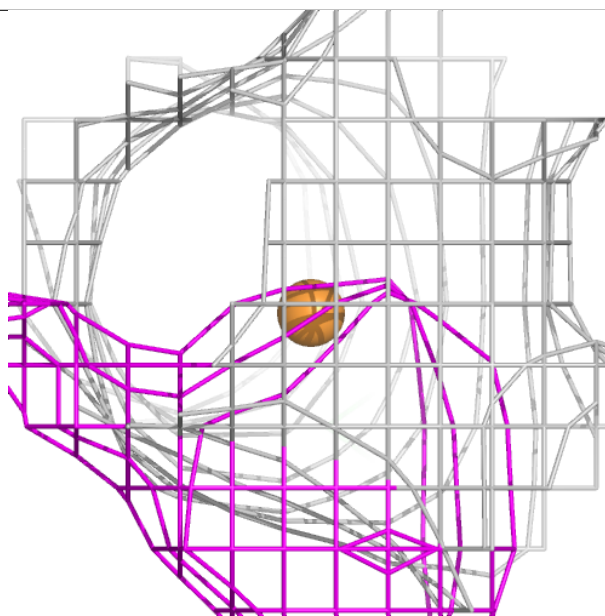
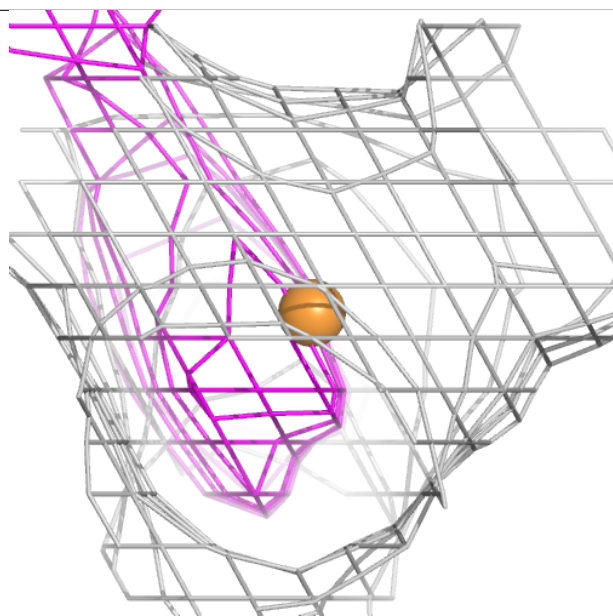
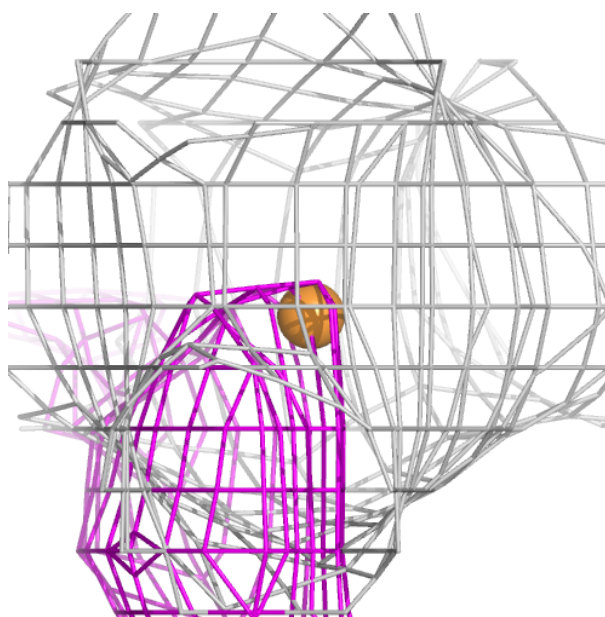
Electron density around CU C 701:

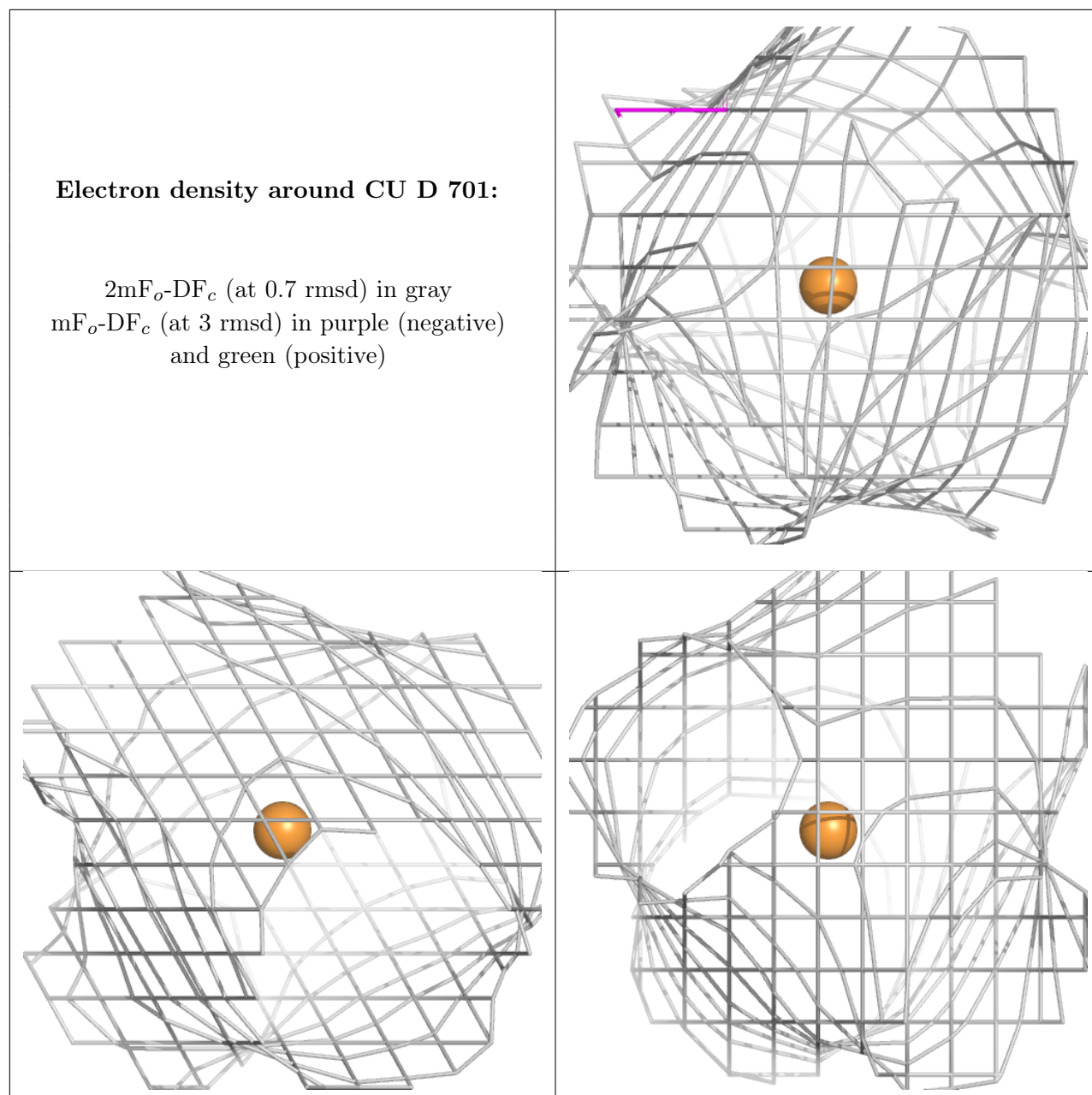
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CU C 702:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.