



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:30 PM UTC

PDB ID : 6LVV / pdb_00006lvv
Title : N, N-dimethylformamidase
Authors : Arya, C.K.; Ramaswamy, S.; Kutti, R.V.; Gurunath, R.
Deposited on : 2020-02-05
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

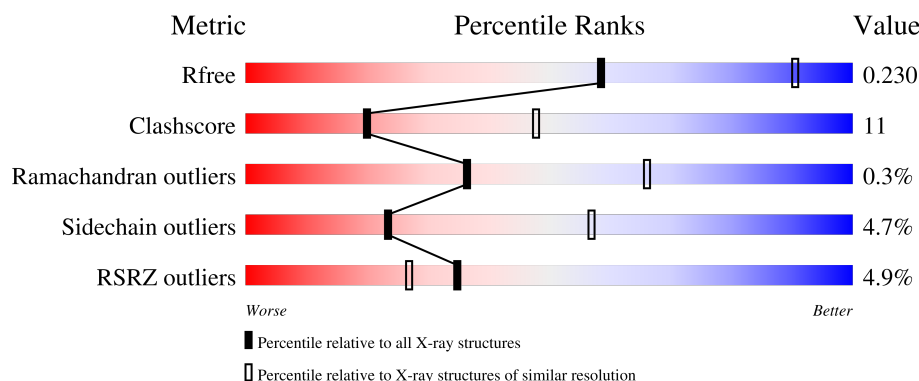
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	775	4% 75% 22% ..
1	C	775	4% 77% 20% ..
1	E	775	5% 75% 21% ..
1	G	775	6% 75% 22% ..
1	I	775	4% 76% 21% ..

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Mol	Chain	Length	Quality of chain
1	K	775	
1	M	775	
1	O	775	
2	B	132	
2	D	132	
2	F	132	
2	H	132	
2	J	132	
2	L	132	
2	N	132	
2	P	132	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 56839 atoms, of which 48 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 N,N-dimethylformamidase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	C	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	E	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	G	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	I	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	K	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	M	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			
1	O	762	Total	C	N	O	S	0	0	0
			5987	3774	1047	1145	21			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	763	LYS	-	expression tag	UNP I6NT79
A	764	LEU	-	expression tag	UNP I6NT79
A	765	ALA	-	expression tag	UNP I6NT79
A	766	ALA	-	expression tag	UNP I6NT79
A	767	ALA	-	expression tag	UNP I6NT79
A	768	LEU	-	expression tag	UNP I6NT79
A	769	GLU	-	expression tag	UNP I6NT79
A	770	HIS	-	expression tag	UNP I6NT79
A	771	HIS	-	expression tag	UNP I6NT79
A	772	HIS	-	expression tag	UNP I6NT79
A	773	HIS	-	expression tag	UNP I6NT79
A	774	HIS	-	expression tag	UNP I6NT79
A	775	HIS	-	expression tag	UNP I6NT79

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Chain	Residue	Modelled	Actual	Comment	Reference
C	763	LYS	-	expression tag	UNP I6NT79
C	764	LEU	-	expression tag	UNP I6NT79
C	765	ALA	-	expression tag	UNP I6NT79
C	766	ALA	-	expression tag	UNP I6NT79
C	767	ALA	-	expression tag	UNP I6NT79
C	768	LEU	-	expression tag	UNP I6NT79
C	769	GLU	-	expression tag	UNP I6NT79
C	770	HIS	-	expression tag	UNP I6NT79
C	771	HIS	-	expression tag	UNP I6NT79
C	772	HIS	-	expression tag	UNP I6NT79
C	773	HIS	-	expression tag	UNP I6NT79
C	774	HIS	-	expression tag	UNP I6NT79
C	775	HIS	-	expression tag	UNP I6NT79
E	763	LYS	-	expression tag	UNP I6NT79
E	764	LEU	-	expression tag	UNP I6NT79
E	765	ALA	-	expression tag	UNP I6NT79
E	766	ALA	-	expression tag	UNP I6NT79
E	767	ALA	-	expression tag	UNP I6NT79
E	768	LEU	-	expression tag	UNP I6NT79
E	769	GLU	-	expression tag	UNP I6NT79
E	770	HIS	-	expression tag	UNP I6NT79
E	771	HIS	-	expression tag	UNP I6NT79
E	772	HIS	-	expression tag	UNP I6NT79
E	773	HIS	-	expression tag	UNP I6NT79
E	774	HIS	-	expression tag	UNP I6NT79
E	775	HIS	-	expression tag	UNP I6NT79
G	763	LYS	-	expression tag	UNP I6NT79
G	764	LEU	-	expression tag	UNP I6NT79
G	765	ALA	-	expression tag	UNP I6NT79
G	766	ALA	-	expression tag	UNP I6NT79
G	767	ALA	-	expression tag	UNP I6NT79
G	768	LEU	-	expression tag	UNP I6NT79
G	769	GLU	-	expression tag	UNP I6NT79
G	770	HIS	-	expression tag	UNP I6NT79
G	771	HIS	-	expression tag	UNP I6NT79
G	772	HIS	-	expression tag	UNP I6NT79
G	773	HIS	-	expression tag	UNP I6NT79
G	774	HIS	-	expression tag	UNP I6NT79
G	775	HIS	-	expression tag	UNP I6NT79
I	763	LYS	-	expression tag	UNP I6NT79
I	764	LEU	-	expression tag	UNP I6NT79
I	765	ALA	-	expression tag	UNP I6NT79

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Chain	Residue	Modelled	Actual	Comment	Reference
I	766	ALA	-	expression tag	UNP I6NT79
I	767	ALA	-	expression tag	UNP I6NT79
I	768	LEU	-	expression tag	UNP I6NT79
I	769	GLU	-	expression tag	UNP I6NT79
I	770	HIS	-	expression tag	UNP I6NT79
I	771	HIS	-	expression tag	UNP I6NT79
I	772	HIS	-	expression tag	UNP I6NT79
I	773	HIS	-	expression tag	UNP I6NT79
I	774	HIS	-	expression tag	UNP I6NT79
I	775	HIS	-	expression tag	UNP I6NT79
K	763	LYS	-	expression tag	UNP I6NT79
K	764	LEU	-	expression tag	UNP I6NT79
K	765	ALA	-	expression tag	UNP I6NT79
K	766	ALA	-	expression tag	UNP I6NT79
K	767	ALA	-	expression tag	UNP I6NT79
K	768	LEU	-	expression tag	UNP I6NT79
K	769	GLU	-	expression tag	UNP I6NT79
K	770	HIS	-	expression tag	UNP I6NT79
K	771	HIS	-	expression tag	UNP I6NT79
K	772	HIS	-	expression tag	UNP I6NT79
K	773	HIS	-	expression tag	UNP I6NT79
K	774	HIS	-	expression tag	UNP I6NT79
K	775	HIS	-	expression tag	UNP I6NT79
M	763	LYS	-	expression tag	UNP I6NT79
M	764	LEU	-	expression tag	UNP I6NT79
M	765	ALA	-	expression tag	UNP I6NT79
M	766	ALA	-	expression tag	UNP I6NT79
M	767	ALA	-	expression tag	UNP I6NT79
M	768	LEU	-	expression tag	UNP I6NT79
M	769	GLU	-	expression tag	UNP I6NT79
M	770	HIS	-	expression tag	UNP I6NT79
M	771	HIS	-	expression tag	UNP I6NT79
M	772	HIS	-	expression tag	UNP I6NT79
M	773	HIS	-	expression tag	UNP I6NT79
M	774	HIS	-	expression tag	UNP I6NT79
M	775	HIS	-	expression tag	UNP I6NT79
O	763	LYS	-	expression tag	UNP I6NT79
O	764	LEU	-	expression tag	UNP I6NT79
O	765	ALA	-	expression tag	UNP I6NT79
O	766	ALA	-	expression tag	UNP I6NT79
O	767	ALA	-	expression tag	UNP I6NT79
O	768	LEU	-	expression tag	UNP I6NT79

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Chain	Residue	Modelled	Actual	Comment	Reference
O	769	GLU	-	expression tag	UNP I6NT79
O	770	HIS	-	expression tag	UNP I6NT79
O	771	HIS	-	expression tag	UNP I6NT79
O	772	HIS	-	expression tag	UNP I6NT79
O	773	HIS	-	expression tag	UNP I6NT79
O	774	HIS	-	expression tag	UNP I6NT79
O	775	HIS	-	expression tag	UNP I6NT79

- Molecule 2 is a protein called N,N-dimethylformamidase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	D	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	F	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	H	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	J	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	L	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	N	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			
2	P	125	Total	C	N	O	S	0	0	0
			1085	687	196	199	3			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

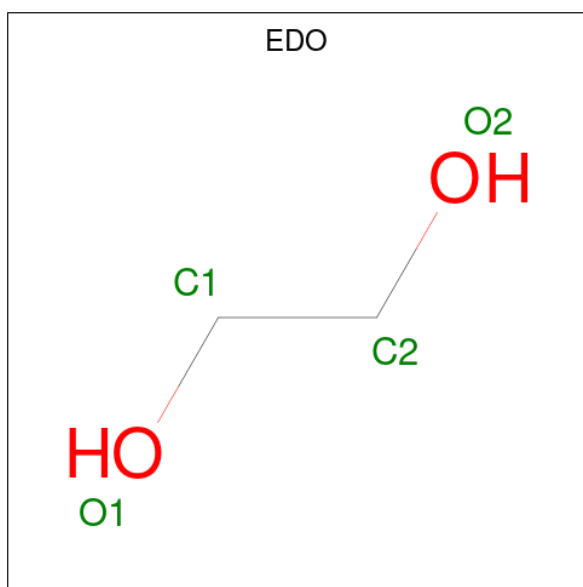
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		
3	E	1	Total	Fe	0	0
			1	1		
3	G	1	Total	Fe	0	0
			1	1		
3	I	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	1	Total	Fe	0	0
			1	1		
3	M	1	Total	Fe	0	0
			1	1		
3	O	1	Total	Fe	0	0
			1	1		

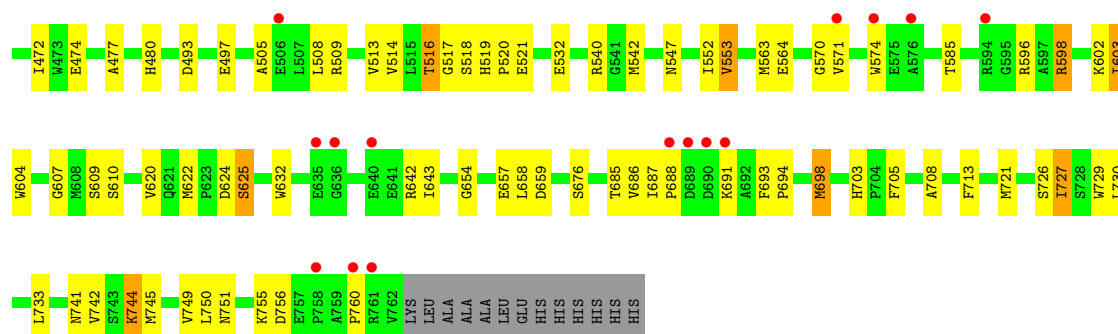
- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



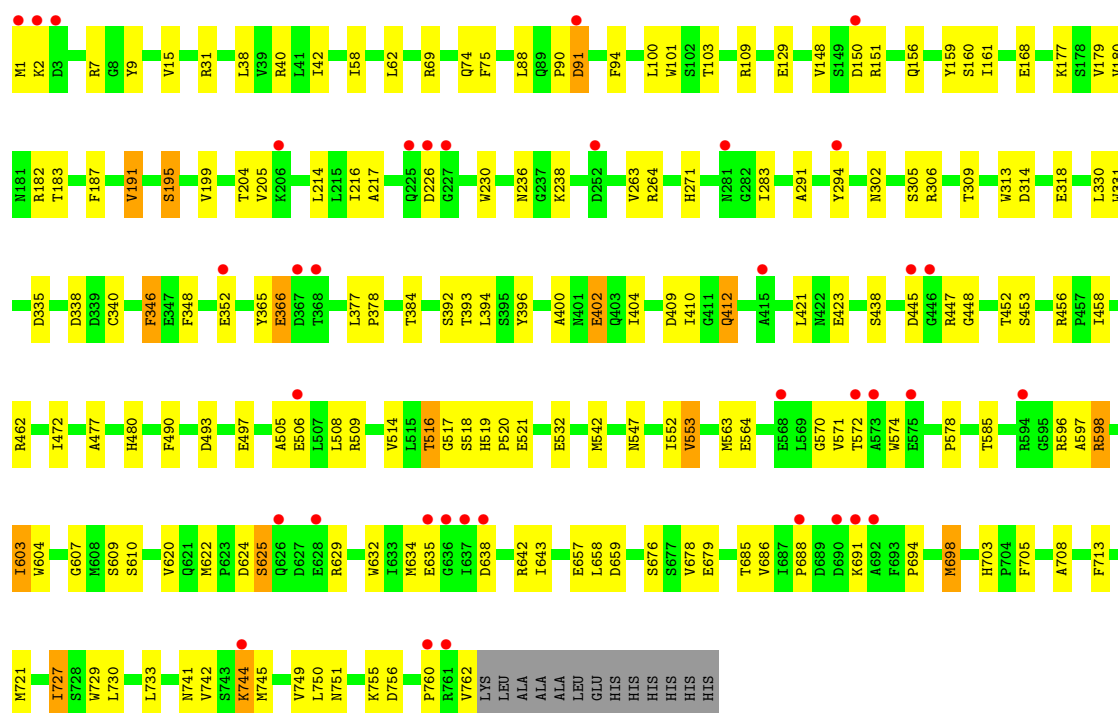
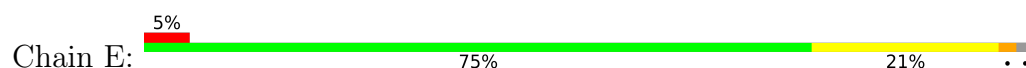
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	F	1	Total	C	H	O	0	0
			10	2	6	2		
4	H	1	Total	C	H	O	0	0
			10	2	6	2		
4	J	1	Total	C	H	O	0	0
			10	2	6	2		
4	L	1	Total	C	H	O	0	0
			10	2	6	2		
4	N	1	Total	C	H	O	0	0
			10	2	6	2		
4	P	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is water.

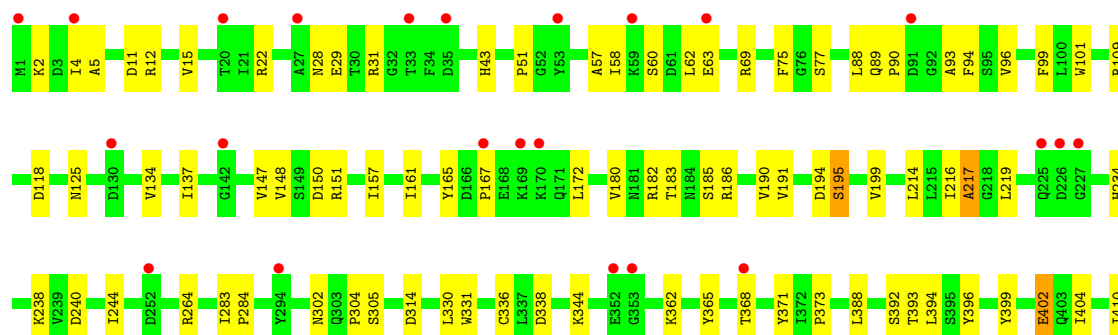
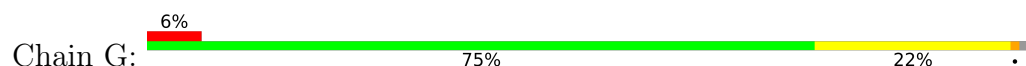
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total 22	O 22	0	0
5	B	1	Total 1	O 1	0	0
5	C	21	Total 21	O 21	0	0
5	E	21	Total 21	O 21	0	0
5	G	22	Total 22	O 22	0	0
5	H	1	Total 1	O 1	0	0
5	I	20	Total 20	O 20	0	0
5	J	1	Total 1	O 1	0	0
5	K	21	Total 21	O 21	0	0
5	M	22	Total 22	O 22	0	0
5	O	23	Total 23	O 23	0	0

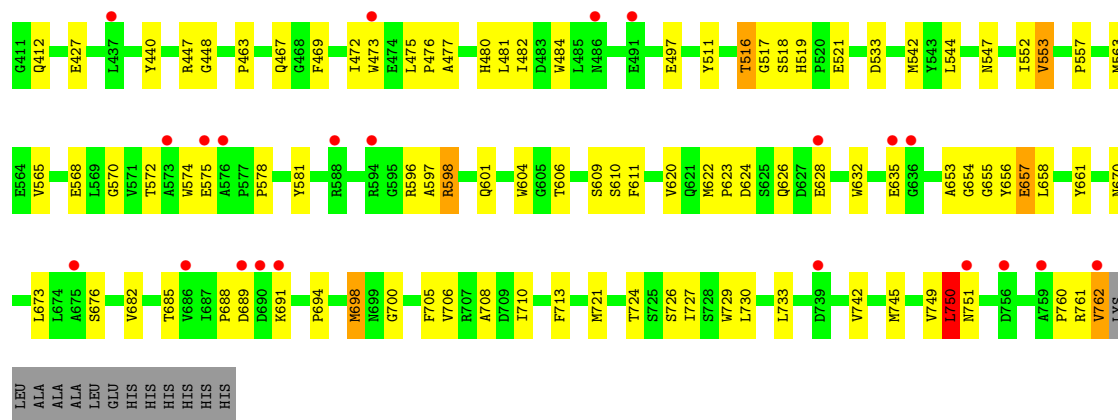


• Molecule 1: N,N-dimethylformamidase large subunit

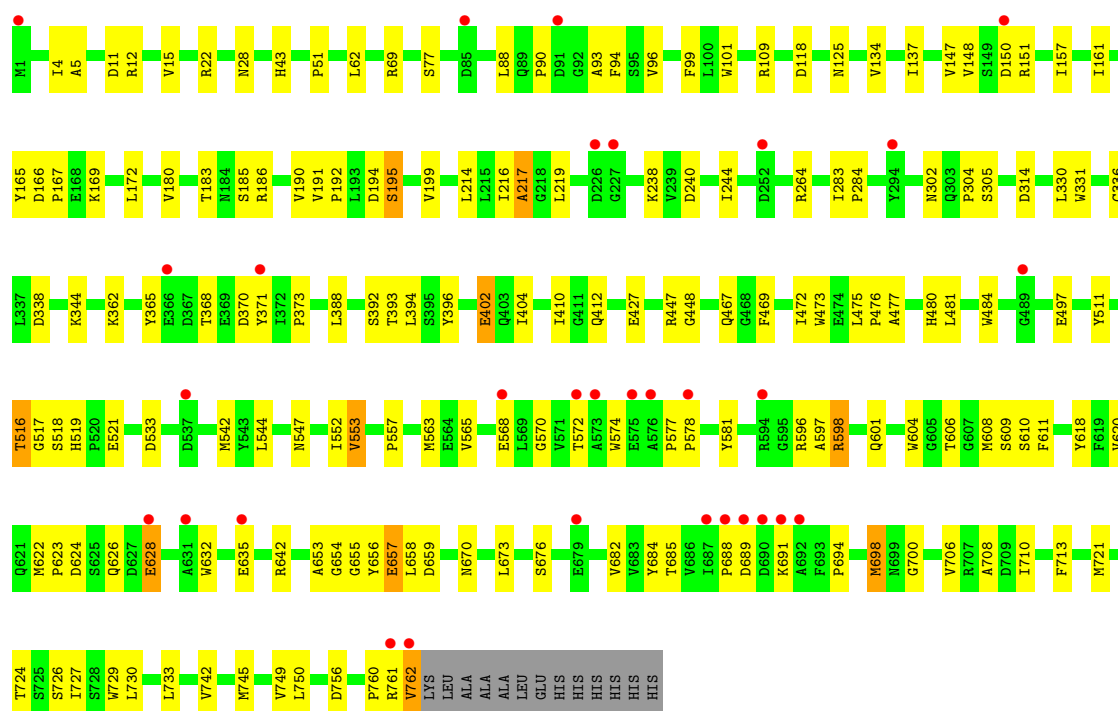
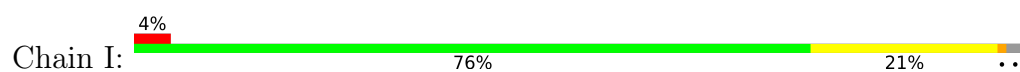


• Molecule 1: N,N-dimethylformamidase large subunit

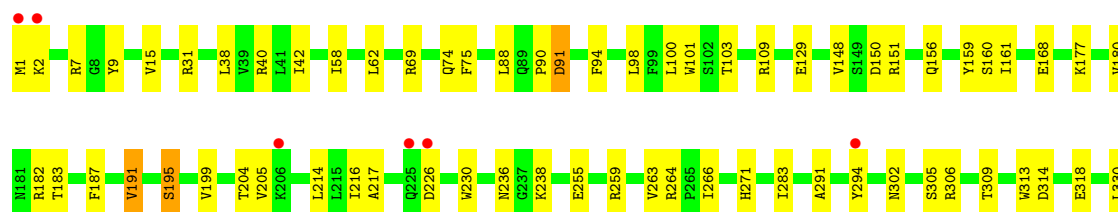
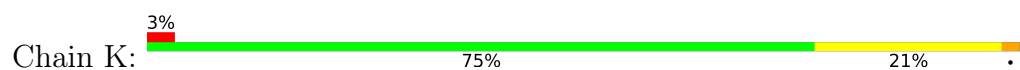


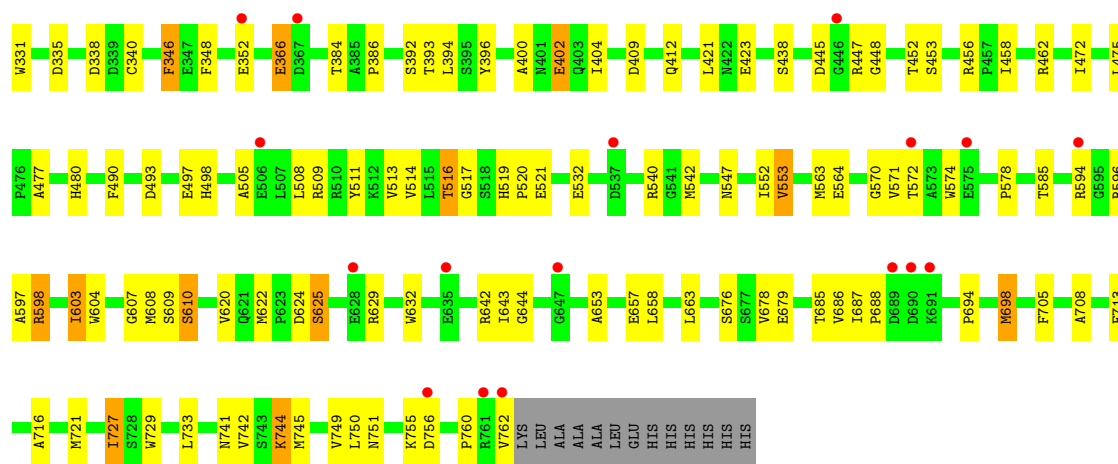


• Molecule 1: N,N-dimethylformamidase large subunit

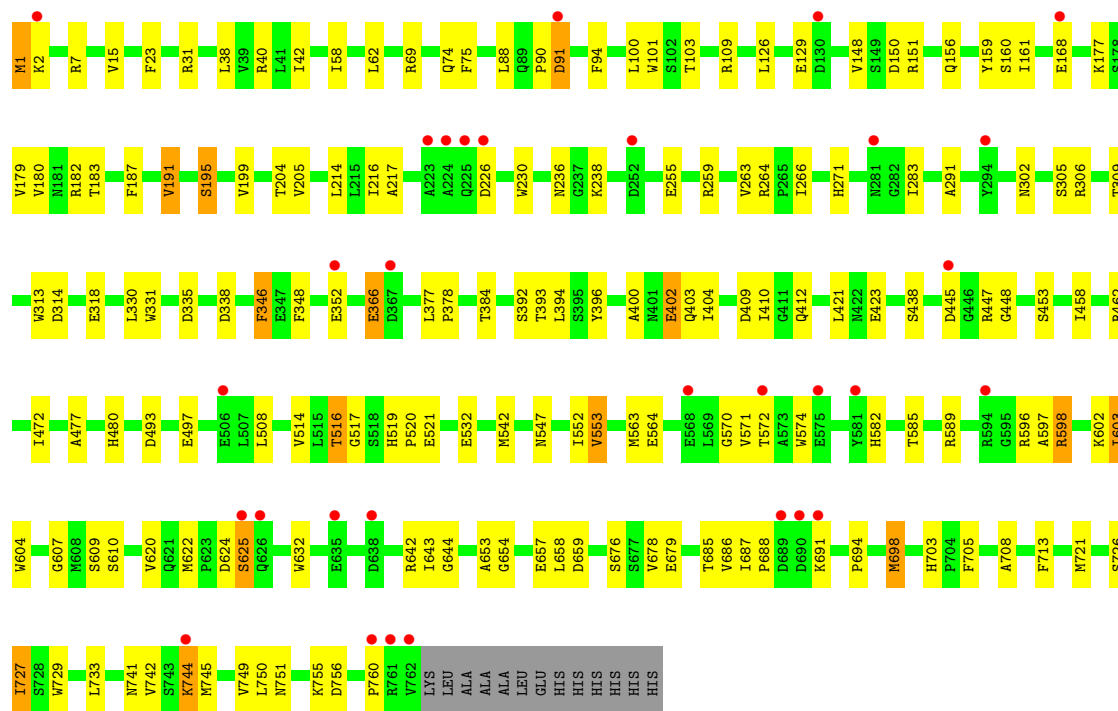
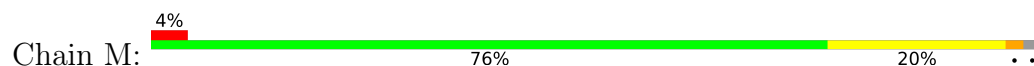


• Molecule 1: N,N-dimethylformamidase large subunit

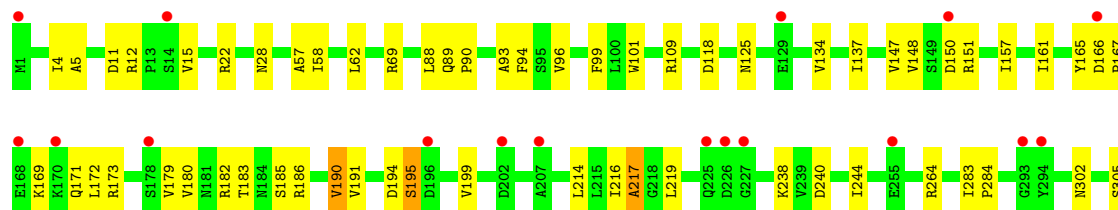
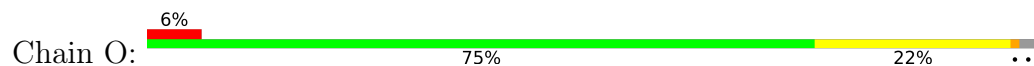


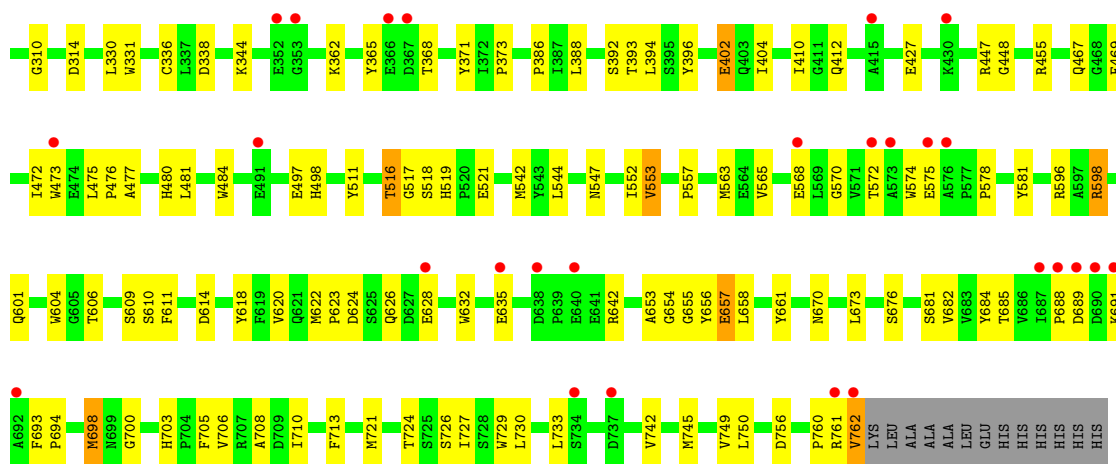


- Molecule 1: N,N-dimethylformamidase large subunit

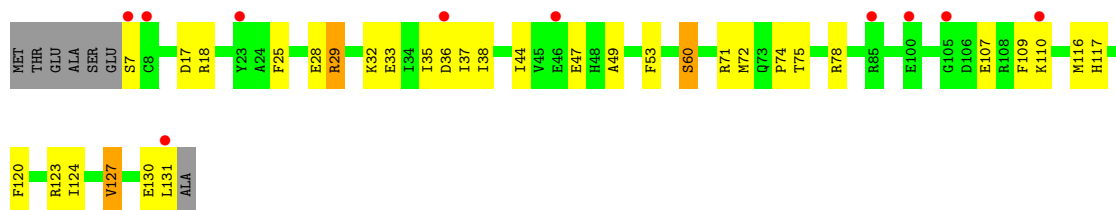


- Molecule 1: N,N-dimethylformamidase large subunit

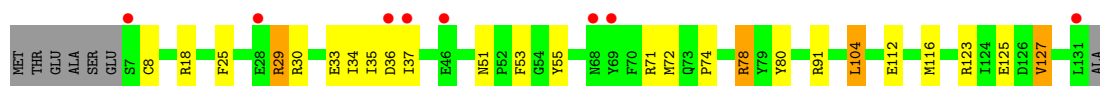
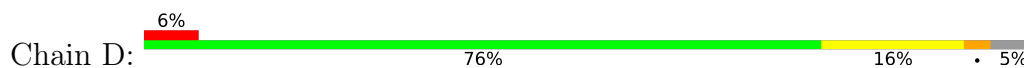




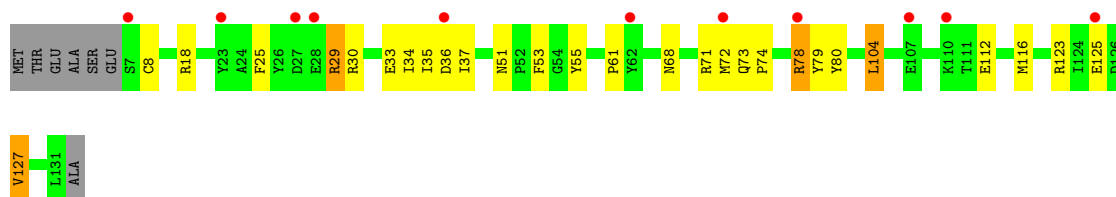
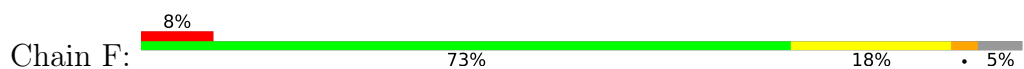
• Molecule 2: N,N-dimethylformamidase small subunit



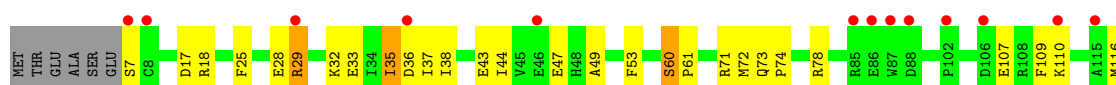
• Molecule 2: N,N-dimethylformamidase small subunit



• Molecule 2: N,N-dimethylformamidase small subunit

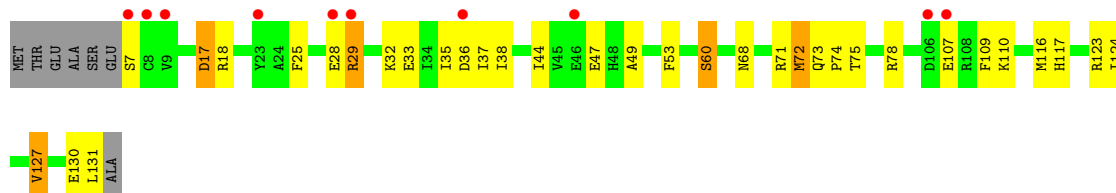


• Molecule 2: N,N-dimethylformamidase small subunit

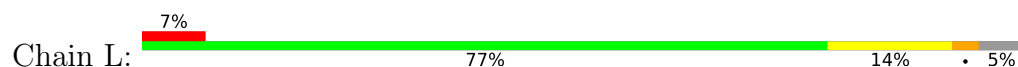




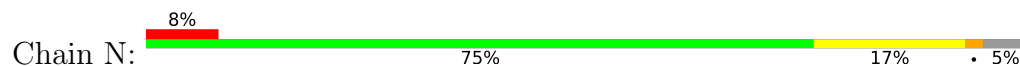
- Molecule 2: N,N-dimethylformamidase small subunit



- Molecule 2: N,N-dimethylformamidase small subunit



- Molecule 2: N,N-dimethylformamidase small subunit



- Molecule 2: N,N-dimethylformamidase small subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	160.51Å 142.55Å 181.49Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	49.47 – 2.80 49.47 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.47-2.80) 99.9 (49.47-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18rc6_3830	Depositor
R, R_{free}	0.227 , 0.267 (Not available) , 0.230	Depositor DCC
R_{free} test set	1924 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	56839	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4942e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, FE

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	0.21	0/6157	0.38	0/8375
1	C	0.28	1/6157 (0.0%)	0.40	0/8375
1	E	0.33	2/6157 (0.0%)	0.41	0/8375
1	G	0.24	1/6157 (0.0%)	0.39	0/8375
1	I	0.24	1/6157 (0.0%)	0.39	0/8375
1	K	0.24	0/6157	0.39	0/8375
1	M	0.24	0/6157	0.39	0/8375
1	O	0.22	0/6157	0.38	0/8375
2	B	0.21	0/1117	0.37	0/1509
2	D	0.20	0/1117	0.38	0/1509
2	F	0.47	1/1117 (0.1%)	0.45	0/1509
2	H	0.37	1/1117 (0.1%)	0.43	0/1509
2	J	0.45	1/1117 (0.1%)	0.45	0/1509
2	L	0.19	0/1117	0.38	0/1509
2	N	0.19	0/1117	0.39	0/1509
2	P	0.49	1/1117 (0.1%)	0.47	0/1509
All	All	0.27	9/58192 (0.0%)	0.40	0/79072

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	348	PHE	C-O	-6.97	1.15	1.24
1	I	370	ASP	C-O	-6.61	1.15	1.23
2	P	73	GLN	C-O	-6.48	1.14	1.23
1	E	410	ILE	C-O	-6.21	1.16	1.24
1	E	412	GLN	C-O	-6.19	1.16	1.24
2	J	75	THR	C-O	-5.91	1.16	1.24
1	G	750	LEU	C-O	-5.77	1.17	1.24
2	F	79	TYR	C-O	-5.75	1.16	1.24
2	H	74	PRO	C-O	-5.28	1.17	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5987	0	5637	148	0
1	C	5987	0	5637	140	0
1	E	5987	0	5637	156	0
1	G	5987	0	5637	147	0
1	I	5987	0	5637	150	0
1	K	5987	0	5637	153	0
1	M	5987	0	5637	149	0
1	O	5987	0	5637	155	0
2	B	1085	0	1010	21	0
2	D	1085	0	1010	19	0
2	F	1085	0	1010	26	0
2	H	1085	0	1010	27	0
2	J	1085	0	1010	24	0
2	L	1085	0	1010	14	0
2	N	1085	0	1010	17	0
2	P	1085	0	1010	25	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
4	B	4	6	6	0	0
4	D	4	6	6	0	0
4	F	4	6	6	0	0
4	H	4	6	6	0	0
4	J	4	6	6	0	0
4	L	4	6	6	0	0
4	N	4	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	4	6	6	0	0
5	A	22	0	0	0	0
5	B	1	0	0	0	0
5	C	21	0	0	1	0
5	E	21	0	0	0	0
5	G	22	0	0	0	0
5	H	1	0	0	1	0
5	I	20	0	0	0	0
5	J	1	0	0	0	0
5	K	21	0	0	4	0
5	M	22	0	0	1	0
5	O	23	0	0	3	0
All	All	56791	48	53224	1252	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1252) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:362:LYS:HE3	1:I:371:TYR:OH	1.44	1.16
1:I:688:PRO:HG2	1:K:688:PRO:HG2	1.28	1.15
1:A:542:MET:HE2	1:A:749:VAL:HG12	1.33	1.10
1:I:542:MET:HE2	1:I:749:VAL:HG12	1.37	1.07
1:E:506:GLU:HG3	1:I:756:ASP:HB2	1.39	1.05
1:G:542:MET:HE2	1:G:749:VAL:HG12	1.35	1.04
1:E:688:PRO:HG2	1:G:688:PRO:HG2	1.35	1.03
1:O:542:MET:HE2	1:O:749:VAL:HG12	1.36	1.03
1:M:688:PRO:HG2	1:O:688:PRO:HG2	1.41	0.99
1:A:688:PRO:HG2	1:C:688:PRO:HG2	1.40	0.98
1:O:394:LEU:HD22	1:O:563:MET:HE2	1.47	0.97
1:C:394:LEU:HD22	1:C:563:MET:HE2	1.47	0.96
1:E:598:ARG:HH11	1:E:598:ARG:HG3	1.29	0.95
1:K:394:LEU:HD22	1:K:563:MET:HE2	1.48	0.95
1:C:598:ARG:HG3	1:C:598:ARG:HH11	1.29	0.95
1:G:394:LEU:HD22	1:G:563:MET:HE2	1.49	0.95
1:K:598:ARG:HG3	1:K:598:ARG:HH11	1.30	0.95
1:M:394:LEU:HD22	1:M:563:MET:HE2	1.48	0.94
1:M:598:ARG:HG3	1:M:598:ARG:HH11	1.29	0.93
1:A:394:LEU:HD22	1:A:563:MET:HE2	1.48	0.93
1:E:394:LEU:HD22	1:E:563:MET:HE2	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:GLN:HB3	2:F:78:ARG:NH2	1.84	0.91
1:I:394:LEU:HD22	1:I:563:MET:HE2	1.49	0.91
1:G:412:GLN:HB3	2:H:78:ARG:HH21	1.38	0.89
1:M:542:MET:HE2	1:M:749:VAL:HG12	1.52	0.89
1:G:412:GLN:HB3	2:H:78:ARG:NH2	1.88	0.89
1:E:412:GLN:HB3	2:F:78:ARG:HH22	1.35	0.89
1:O:412:GLN:HB3	2:P:78:ARG:HH21	1.39	0.88
1:I:412:GLN:HB3	2:J:78:ARG:NH2	1.89	0.88
1:E:542:MET:HE2	1:E:749:VAL:HG12	1.55	0.88
1:G:542:MET:HE1	1:G:750:LEU:HA	1.55	0.87
1:O:412:GLN:HB3	2:P:78:ARG:NH2	1.89	0.86
1:I:412:GLN:HB3	2:J:78:ARG:HH21	1.39	0.86
1:C:542:MET:HE2	1:C:749:VAL:HG12	1.55	0.86
1:E:506:GLU:CG	1:I:756:ASP:HB2	2.06	0.85
1:A:542:MET:HE1	1:A:750:LEU:HA	1.58	0.84
1:I:542:MET:HE1	1:I:750:LEU:HA	1.59	0.84
1:K:542:MET:HE2	1:K:749:VAL:HG12	1.59	0.83
1:O:542:MET:HE1	1:O:750:LEU:HA	1.60	0.83
1:M:542:MET:HE1	1:M:750:LEU:HA	1.61	0.83
1:M:622:MET:HA	1:M:622:MET:HE2	1.61	0.82
1:E:542:MET:HE1	1:E:750:LEU:HA	1.62	0.82
1:K:542:MET:HE1	1:K:750:LEU:HA	1.61	0.81
1:G:670:ASN:HB2	1:G:762:VAL:HG11	1.63	0.81
1:K:472:ILE:HD11	1:K:480:HIS:CE1	2.15	0.81
1:O:670:ASN:HB2	1:O:762:VAL:HG11	1.63	0.81
1:C:622:MET:HE2	1:C:622:MET:HA	1.62	0.81
1:I:670:ASN:HB2	1:I:762:VAL:HG11	1.62	0.80
1:C:542:MET:HE1	1:C:750:LEU:HA	1.61	0.80
1:E:472:ILE:HD11	1:E:480:HIS:CE1	2.16	0.80
1:M:472:ILE:HD11	1:M:480:HIS:CE1	2.17	0.80
1:O:386:PRO:HA	5:O:917:HOH:O	1.81	0.80
1:I:412:GLN:HE22	2:J:123:ARG:HH22	1.30	0.80
1:G:412:GLN:HE22	2:H:123:ARG:HH22	1.30	0.79
1:A:670:ASN:HB2	1:A:762:VAL:HG11	1.63	0.79
1:C:542:MET:HE1	1:C:750:LEU:CA	2.12	0.79
1:E:744:LYS:HA	1:E:744:LYS:HE3	1.65	0.79
1:C:472:ILE:HD11	1:C:480:HIS:CE1	2.17	0.79
1:A:412:GLN:HE22	2:B:123:ARG:HH22	1.31	0.78
1:M:542:MET:HE1	1:M:750:LEU:CA	2.13	0.78
1:K:622:MET:HA	1:K:622:MET:HE2	1.64	0.78
1:K:542:MET:HE1	1:K:750:LEU:CA	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:542:MET:HE1	1:O:750:LEU:CA	2.14	0.78
1:E:622:MET:HE2	1:E:622:MET:HA	1.66	0.78
1:A:542:MET:HE1	1:A:750:LEU:CA	2.13	0.77
1:G:542:MET:HE1	1:G:750:LEU:CA	2.15	0.77
1:K:183:THR:HG21	1:K:314:ASP:HA	1.67	0.77
1:E:542:MET:HE1	1:E:750:LEU:CA	2.14	0.77
1:M:744:LYS:HE3	1:M:744:LYS:HA	1.66	0.77
1:I:542:MET:HE1	1:I:750:LEU:CA	2.14	0.77
1:C:744:LYS:HE3	1:C:744:LYS:HA	1.67	0.76
1:O:412:GLN:HE22	2:P:123:ARG:HH22	1.31	0.76
1:A:394:LEU:HA	1:A:563:MET:HE1	1.66	0.76
1:I:688:PRO:HG2	1:K:688:PRO:CG	2.12	0.76
1:M:516:THR:HG22	1:M:517:GLY:O	1.86	0.76
1:K:744:LYS:HE3	1:K:744:LYS:HA	1.67	0.76
1:E:516:THR:HG22	1:E:517:GLY:O	1.87	0.75
1:C:598:ARG:HG3	1:C:598:ARG:NH1	2.00	0.75
1:A:394:LEU:CA	1:A:563:MET:HE1	2.16	0.75
1:E:688:PRO:CG	1:G:688:PRO:HG2	2.16	0.75
1:O:610:SER:HB2	1:O:685:THR:O	1.86	0.75
1:K:598:ARG:HG3	1:K:598:ARG:NH1	2.00	0.74
1:C:101:TRP:CZ2	1:C:156:GLN:HG2	2.22	0.74
1:G:610:SER:HB2	1:G:685:THR:O	1.87	0.74
1:M:183:THR:HG21	1:M:314:ASP:HA	1.70	0.74
1:C:183:THR:HG21	1:C:314:ASP:HA	1.70	0.74
1:C:516:THR:HG22	1:C:517:GLY:O	1.88	0.74
1:G:394:LEU:HA	1:G:563:MET:HE1	1.69	0.74
1:E:101:TRP:CZ2	1:E:156:GLN:HG2	2.23	0.74
1:M:101:TRP:CZ2	1:M:156:GLN:HG2	2.23	0.74
1:K:101:TRP:CZ2	1:K:156:GLN:HG2	2.23	0.73
1:K:516:THR:HG22	1:K:517:GLY:O	1.87	0.73
1:O:394:LEU:HA	1:O:563:MET:HE1	1.69	0.73
1:O:394:LEU:CA	1:O:563:MET:HE1	2.18	0.73
1:G:472:ILE:HD11	1:G:480:HIS:CE1	2.23	0.73
2:J:73:GLN:O	2:J:78:ARG:NH1	2.20	0.73
2:J:68:ASN:O	2:J:72:MET:HG2	1.88	0.73
1:E:183:THR:HG21	1:E:314:ASP:HA	1.71	0.73
1:A:516:THR:HG23	1:A:517:GLY:O	1.89	0.73
1:A:610:SER:HB2	1:A:685:THR:O	1.88	0.73
1:K:409:ASP:OD2	2:L:74:PRO:HA	1.89	0.73
1:I:394:LEU:HA	1:I:563:MET:HE1	1.70	0.72
1:K:386:PRO:HA	5:K:907:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:688:PRO:CG	1:K:688:PRO:HG2	2.15	0.72
1:I:610:SER:HB2	1:I:685:THR:O	1.89	0.72
1:G:516:THR:HG23	1:G:517:GLY:O	1.90	0.72
2:N:35:ILE:HD11	2:N:127:VAL:HG13	1.72	0.72
1:I:394:LEU:CA	1:I:563:MET:HE1	2.19	0.72
2:F:35:ILE:HD11	2:F:127:VAL:HG13	1.72	0.72
1:I:516:THR:HG23	1:I:517:GLY:O	1.90	0.72
1:M:409:ASP:OD2	2:N:74:PRO:HA	1.90	0.71
1:G:553:VAL:HG13	1:G:563:MET:HG3	1.72	0.71
2:F:68:ASN:O	2:F:72:MET:HG2	1.91	0.71
1:G:394:LEU:CA	1:G:563:MET:HE1	2.20	0.71
1:C:409:ASP:OD2	2:D:74:PRO:HA	1.91	0.71
1:I:4:ILE:HB	1:I:427:GLU:HG3	1.72	0.71
1:O:472:ILE:HD11	1:O:480:HIS:CE1	2.25	0.71
1:A:5:ALA:HA	1:A:28:ASN:ND2	2.06	0.71
1:O:516:THR:HG23	1:O:517:GLY:O	1.91	0.71
1:M:23:PHE:HB2	1:M:346:PHE:CE1	2.25	0.71
1:I:371:TYR:O	1:I:373:PRO:HD3	1.92	0.70
1:I:362:LYS:CE	1:I:371:TYR:OH	2.33	0.70
1:A:4:ILE:HB	1:A:427:GLU:HG3	1.74	0.70
1:I:5:ALA:HA	1:I:28:ASN:ND2	2.07	0.70
1:A:552:ILE:CD1	1:A:596:ARG:HG3	2.22	0.70
1:O:553:VAL:HG13	1:O:563:MET:HG3	1.74	0.70
2:D:35:ILE:HD11	2:D:127:VAL:HG13	1.73	0.70
1:O:4:ILE:HB	1:O:427:GLU:HG3	1.72	0.70
1:O:88:LEU:HD13	1:O:214:LEU:HD13	1.73	0.69
1:A:472:ILE:HD11	1:A:480:HIS:CE1	2.28	0.69
1:G:5:ALA:HA	1:G:28:ASN:ND2	2.07	0.69
1:I:472:ILE:HD11	1:I:480:HIS:CE1	2.28	0.69
1:M:598:ARG:HG3	1:M:598:ARG:NH1	2.00	0.69
2:L:35:ILE:HD11	2:L:127:VAL:HG13	1.73	0.69
1:A:553:VAL:HG13	1:A:563:MET:HG3	1.75	0.68
1:E:412:GLN:CB	2:F:78:ARG:NH2	2.56	0.68
1:I:553:VAL:HG13	1:I:563:MET:HG3	1.74	0.68
1:G:4:ILE:HB	1:G:427:GLU:HG3	1.73	0.68
1:I:552:ILE:CD1	1:I:596:ARG:HG3	2.23	0.68
1:O:5:ALA:HA	1:O:28:ASN:ND2	2.07	0.68
1:O:552:ILE:CD1	1:O:596:ARG:HG3	2.23	0.68
1:A:88:LEU:HD13	1:A:214:LEU:HD13	1.74	0.67
1:C:642:ARG:O	1:C:741:ASN:ND2	2.27	0.67
1:I:88:LEU:HD13	1:I:214:LEU:HD13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:TRP:CE2	1:A:760:PRO:HG2	2.29	0.67
1:C:394:LEU:CA	1:C:563:MET:HE1	2.25	0.67
1:E:394:LEU:HD22	1:E:563:MET:CE	2.25	0.67
1:E:598:ARG:HG3	1:E:598:ARG:NH1	1.99	0.67
1:G:552:ILE:CD1	1:G:596:ARG:HG3	2.24	0.67
1:G:632:TRP:CE2	1:G:760:PRO:HG2	2.29	0.67
1:I:632:TRP:CE2	1:I:760:PRO:HG2	2.30	0.67
1:K:642:ARG:O	1:K:741:ASN:ND2	2.28	0.67
1:G:412:GLN:HG2	2:H:71:ARG:HG2	1.77	0.66
1:E:688:PRO:HG2	1:G:688:PRO:CG	2.19	0.66
1:O:632:TRP:CE2	1:O:760:PRO:HG2	2.30	0.66
1:G:88:LEU:HD13	1:G:214:LEU:HD13	1.75	0.66
1:K:412:GLN:HE22	2:L:123:ARG:HH22	1.44	0.66
1:M:91:ASP:OD1	1:M:91:ASP:N	2.25	0.66
1:I:552:ILE:HD11	1:I:596:ARG:HG3	1.78	0.66
1:E:744:LYS:HE3	1:E:744:LYS:CA	2.26	0.65
1:E:283:ILE:HG23	1:E:283:ILE:O	1.96	0.65
1:G:710:ILE:HD13	1:G:745:MET:HE1	1.76	0.65
1:M:394:LEU:CA	1:M:563:MET:HE1	2.26	0.65
1:M:409:ASP:O	2:N:78:ARG:NH2	2.30	0.65
1:M:412:GLN:HE22	2:N:123:ARG:HH22	1.43	0.65
1:K:394:LEU:CA	1:K:563:MET:HE1	2.27	0.65
2:H:33:GLU:O	2:H:37:ILE:HG13	1.97	0.65
1:C:412:GLN:HE22	2:D:123:ARG:HH22	1.45	0.64
1:E:642:ARG:O	1:E:741:ASN:ND2	2.30	0.64
1:O:394:LEU:HD22	1:O:563:MET:CE	2.25	0.64
1:A:552:ILE:HD11	1:A:596:ARG:HG3	1.79	0.64
1:I:710:ILE:HD13	1:I:745:MET:HE1	1.79	0.64
1:K:394:LEU:O	1:K:563:MET:HE1	1.98	0.64
1:M:642:ARG:O	1:M:741:ASN:ND2	2.30	0.64
1:M:744:LYS:HE3	1:M:744:LYS:CA	2.27	0.64
1:C:519:HIS:HE1	1:C:547:ASN:HD22	1.46	0.64
1:K:394:LEU:HD22	1:K:563:MET:CE	2.26	0.64
1:K:519:HIS:HE1	1:K:547:ASN:HD22	1.46	0.64
1:G:516:THR:HG22	1:G:544:LEU:H	1.63	0.64
2:J:33:GLU:O	2:J:37:ILE:HG13	1.97	0.64
1:M:394:LEU:O	1:M:563:MET:HE1	1.98	0.64
1:O:151:ARG:HG2	1:O:195:SER:HA	1.79	0.64
1:K:409:ASP:O	2:L:78:ARG:NH2	2.31	0.64
2:P:33:GLU:O	2:P:37:ILE:HG13	1.98	0.64
1:C:283:ILE:HG23	1:C:283:ILE:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:394:LEU:CA	1:E:563:MET:HE1	2.27	0.64
1:O:516:THR:HG22	1:O:544:LEU:H	1.63	0.64
2:B:33:GLU:O	2:B:37:ILE:HG13	1.97	0.64
1:M:302:ASN:HA	1:M:338:ASP:OD1	1.97	0.63
1:C:409:ASP:O	2:D:78:ARG:NH2	2.31	0.63
1:C:552:ILE:CD1	1:C:596:ARG:HG3	2.28	0.63
1:C:394:LEU:O	1:C:563:MET:HE1	1.98	0.63
1:I:519:HIS:HE1	1:I:547:ASN:HD22	1.44	0.63
1:O:552:ILE:HD11	1:O:596:ARG:HG3	1.80	0.63
1:E:91:ASP:OD1	1:E:91:ASP:N	2.26	0.63
1:C:302:ASN:HA	1:C:338:ASP:OD1	1.98	0.63
1:G:412:GLN:CB	2:H:78:ARG:HH21	2.12	0.63
1:C:744:LYS:HE3	1:C:744:LYS:CA	2.28	0.63
1:G:552:ILE:HD11	1:G:596:ARG:HG3	1.81	0.63
1:K:283:ILE:O	1:K:283:ILE:HG23	1.98	0.63
1:K:744:LYS:HE3	1:K:744:LYS:CA	2.28	0.63
1:O:412:GLN:HG2	2:P:71:ARG:HG2	1.80	0.63
1:I:151:ARG:HG2	1:I:195:SER:HA	1.81	0.63
1:O:412:GLN:CB	2:P:78:ARG:HH21	2.12	0.63
1:C:394:LEU:HD22	1:C:563:MET:CE	2.27	0.62
1:M:283:ILE:HG23	1:M:283:ILE:O	1.99	0.62
1:E:519:HIS:HE1	1:E:547:ASN:HD22	1.45	0.62
1:O:519:HIS:HE1	1:O:547:ASN:HD22	1.45	0.62
1:I:157:ILE:HD13	1:I:185:SER:HB3	1.80	0.62
1:I:412:GLN:HG2	2:J:71:ARG:HG2	1.82	0.62
1:A:598:ARG:HG3	1:A:598:ARG:HH11	1.64	0.62
1:K:75:PHE:CE2	1:K:335:ASP:HA	2.35	0.62
1:O:710:ILE:HD13	1:O:745:MET:HE1	1.81	0.62
1:G:519:HIS:HE1	1:G:547:ASN:HD22	1.46	0.62
1:K:305:SER:HB2	1:K:331:TRP:HB3	1.82	0.62
1:K:552:ILE:CD1	1:K:596:ARG:HG3	2.29	0.62
1:A:412:GLN:HG2	2:B:71:ARG:HG2	1.81	0.62
1:E:75:PHE:CE2	1:E:335:ASP:HA	2.34	0.62
1:K:511:TYR:HA	5:K:907:HOH:O	2.00	0.62
1:O:622:MET:HE2	1:O:622:MET:HA	1.81	0.62
1:G:151:ARG:HG2	1:G:195:SER:HA	1.81	0.62
1:I:710:ILE:HD13	1:I:745:MET:CE	2.30	0.62
1:A:676:SER:HA	1:A:708:ALA:O	2.00	0.61
1:E:394:LEU:O	1:E:563:MET:HE1	2.00	0.61
1:K:183:THR:CG2	1:K:314:ASP:HA	2.28	0.61
1:G:284:PRO:HB2	1:G:557:PRO:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:710:ILE:HD13	1:G:745:MET:CE	2.30	0.61
1:O:169:LYS:HE3	1:O:173:ARG:HH12	1.64	0.61
1:A:598:ARG:HD3	1:C:182:ARG:O	2.01	0.61
1:A:519:HIS:HE1	1:A:547:ASN:HD22	1.47	0.61
1:I:284:PRO:HB2	1:I:557:PRO:HG2	1.81	0.61
1:K:751:ASN:O	1:K:755:LYS:HG3	1.99	0.61
1:A:151:ARG:HG2	1:A:195:SER:HA	1.82	0.61
1:C:305:SER:HB2	1:C:331:TRP:HB3	1.83	0.61
1:G:598:ARG:HG3	1:G:598:ARG:HH11	1.64	0.61
1:K:302:ASN:HA	1:K:338:ASP:OD1	2.00	0.61
1:C:394:LEU:HA	1:C:563:MET:HE1	1.82	0.61
1:A:622:MET:HA	1:A:622:MET:HE2	1.81	0.61
1:C:75:PHE:CE2	1:C:335:ASP:HA	2.36	0.61
1:G:542:MET:HE1	1:G:750:LEU:N	2.15	0.61
1:G:654:GLY:HA2	1:G:726:SER:OG	2.01	0.61
1:I:412:GLN:CB	2:J:78:ARG:HH21	2.11	0.61
1:M:751:ASN:O	1:M:755:LYS:HG3	2.00	0.61
1:A:542:MET:HE2	1:A:749:VAL:CG1	2.22	0.61
1:A:99:PHE:HB2	1:A:240:ASP:HB3	1.83	0.60
1:C:542:MET:CE	1:C:750:LEU:HA	2.30	0.60
1:E:751:ASN:O	1:E:755:LYS:HG3	2.00	0.60
1:I:99:PHE:HB2	1:I:240:ASP:HB3	1.83	0.60
1:M:183:THR:CG2	1:M:314:ASP:HA	2.30	0.60
1:I:598:ARG:HG3	1:I:598:ARG:HH11	1.64	0.60
2:P:72:MET:HG3	2:P:72:MET:O	2.00	0.60
1:K:542:MET:CE	1:K:750:LEU:HA	2.30	0.60
1:M:703:HIS:CD2	2:P:72:MET:HE1	2.36	0.60
1:O:598:ARG:HG3	1:O:598:ARG:HH11	1.65	0.60
1:A:516:THR:HG22	1:A:544:LEU:H	1.66	0.60
1:G:676:SER:HA	1:G:708:ALA:O	2.00	0.60
1:I:676:SER:HA	1:I:708:ALA:O	2.01	0.60
1:K:266:ILE:HD13	1:O:12:ARG:CB	2.32	0.60
1:M:519:HIS:HE1	1:M:547:ASN:HD22	1.47	0.60
1:M:552:ILE:CD1	1:M:596:ARG:HG3	2.30	0.60
1:A:284:PRO:HB2	1:A:557:PRO:HG2	1.83	0.60
1:A:729:TRP:HH2	1:A:745:MET:HE2	1.65	0.60
1:E:183:THR:CG2	1:E:314:ASP:HA	2.31	0.60
1:E:542:MET:CE	1:E:750:LEU:HA	2.31	0.60
1:E:552:ILE:CD1	1:E:596:ARG:HG3	2.31	0.60
1:A:157:ILE:HD13	1:A:185:SER:HB3	1.82	0.60
1:E:305:SER:HB2	1:E:331:TRP:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:622:MET:HE2	1:G:622:MET:HA	1.83	0.60
1:M:75:PHE:CE2	1:M:335:ASP:HA	2.37	0.60
1:C:91:ASP:OD1	1:C:91:ASP:N	2.25	0.60
1:G:93:ALA:HB2	1:G:167:PRO:HD2	1.83	0.59
1:I:516:THR:HG22	1:I:544:LEU:H	1.66	0.59
1:I:622:MET:HE2	1:I:622:MET:HA	1.83	0.59
1:M:182:ARG:O	1:O:598:ARG:HD3	2.02	0.59
1:O:676:SER:HA	1:O:708:ALA:O	2.01	0.59
1:M:305:SER:HB2	1:M:331:TRP:HB3	1.84	0.59
1:M:394:LEU:HA	1:M:563:MET:HE1	1.84	0.59
1:C:183:THR:CG2	1:C:314:ASP:HA	2.31	0.59
2:H:73:GLN:O	2:H:78:ARG:NH1	2.34	0.59
1:M:394:LEU:HD22	1:M:563:MET:CE	2.28	0.59
1:M:542:MET:CE	1:M:750:LEU:HA	2.31	0.59
1:O:655:GLY:O	1:O:656:TYR:HB2	2.03	0.59
1:A:93:ALA:HB2	1:A:167:PRO:HD2	1.85	0.59
2:F:72:MET:HG3	2:F:72:MET:O	2.02	0.59
1:I:392:SER:HA	1:I:497:GLU:CD	2.28	0.59
1:A:710:ILE:HD13	1:A:745:MET:HE1	1.85	0.59
1:C:643:ILE:HD13	1:C:745:MET:HE2	1.84	0.59
1:C:751:ASN:O	1:C:755:LYS:HG3	2.02	0.59
1:O:157:ILE:HD13	1:O:185:SER:HB3	1.85	0.59
1:A:394:LEU:HD22	1:A:563:MET:CE	2.27	0.59
1:E:394:LEU:HA	1:E:563:MET:HE1	1.84	0.59
2:H:123:ARG:O	2:H:127:VAL:HG12	2.03	0.59
2:D:25:PHE:CZ	2:D:29:ARG:HD2	2.37	0.59
1:G:157:ILE:HD13	1:G:185:SER:HB3	1.85	0.59
1:G:392:SER:HA	1:G:497:GLU:CD	2.27	0.59
1:M:688:PRO:CG	1:O:688:PRO:HG2	2.25	0.59
1:C:657:GLU:HG3	1:C:727:ILE:HD12	1.85	0.58
1:K:609:SER:OG	1:K:705:PHE:O	2.21	0.58
1:A:568:GLU:HG3	1:A:581:TYR:CE1	2.39	0.58
1:E:302:ASN:HA	1:E:338:ASP:OD1	2.02	0.58
1:I:654:GLY:HA2	1:I:726:SER:OG	2.02	0.58
1:E:2:LYS:HD3	1:E:423:GLU:OE1	2.04	0.58
1:K:394:LEU:HA	1:K:563:MET:HE1	1.85	0.58
1:O:710:ILE:HD13	1:O:745:MET:CE	2.34	0.58
2:B:123:ARG:O	2:B:127:VAL:HG12	2.04	0.58
2:P:123:ARG:O	2:P:127:VAL:HG12	2.04	0.58
1:A:624:ASP:OD2	2:D:18:ARG:HD3	2.04	0.58
1:K:657:GLU:HG3	1:K:727:ILE:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:284:PRO:HB2	1:O:557:PRO:HG2	1.84	0.58
1:C:216:ILE:O	1:C:217:ALA:HB3	2.03	0.58
1:I:362:LYS:HE3	1:I:371:TYR:CZ	2.38	0.58
1:O:392:SER:HA	1:O:497:GLU:CD	2.28	0.58
1:C:552:ILE:HD11	1:C:596:ARG:HG3	1.84	0.58
2:N:25:PHE:CZ	2:N:29:ARG:HD2	2.39	0.58
1:O:93:ALA:HB2	1:O:167:PRO:HD2	1.85	0.58
1:A:392:SER:HA	1:A:497:GLU:CD	2.29	0.57
1:E:657:GLU:HG3	1:E:727:ILE:HD12	1.85	0.57
1:G:655:GLY:O	1:G:656:TYR:HB2	2.04	0.57
1:I:655:GLY:O	1:I:656:TYR:HB2	2.04	0.57
1:K:552:ILE:HD11	1:K:596:ARG:HG3	1.85	0.57
1:A:710:ILE:HD13	1:A:745:MET:CE	2.34	0.57
1:M:552:ILE:HD11	1:M:596:ARG:HG3	1.85	0.57
2:P:53:PHE:CZ	2:P:116:MET:HE1	2.39	0.57
2:F:25:PHE:CZ	2:F:29:ARG:HD2	2.39	0.57
1:K:2:LYS:HD3	1:K:423:GLU:OE1	2.04	0.57
1:M:394:LEU:CD2	1:M:563:MET:HE2	2.31	0.57
1:G:99:PHE:HB2	1:G:240:ASP:HB3	1.86	0.57
1:I:542:MET:CE	1:I:750:LEU:HA	2.34	0.57
1:O:99:PHE:HB2	1:O:240:ASP:HB3	1.86	0.57
1:A:194:ASP:HB2	2:B:7:SER:N	2.20	0.57
1:G:729:TRP:HH2	1:G:745:MET:HE2	1.69	0.57
1:K:183:THR:HG21	1:K:314:ASP:CA	2.35	0.57
1:O:729:TRP:CZ2	1:O:742:VAL:HG13	2.40	0.57
1:A:654:GLY:HA2	1:A:726:SER:OG	2.04	0.57
1:C:2:LYS:HD3	1:C:423:GLU:OE1	2.04	0.57
1:I:518:SER:HB3	1:I:730:LEU:HD12	1.86	0.57
1:M:2:LYS:HD3	1:M:423:GLU:OE1	2.05	0.57
1:M:694:PRO:HA	1:M:698:MET:HE2	1.87	0.57
1:C:694:PRO:HA	1:C:698:MET:HE2	1.86	0.56
1:E:609:SER:OG	1:E:705:PHE:O	2.22	0.56
2:J:123:ARG:O	2:J:127:VAL:HG12	2.05	0.56
1:M:676:SER:HA	1:M:708:ALA:O	2.05	0.56
1:C:609:SER:OG	1:C:705:PHE:O	2.22	0.56
1:E:109:ARG:HG3	1:E:129:GLU:HG2	1.87	0.56
1:O:654:GLY:HA2	1:O:726:SER:OG	2.05	0.56
1:A:394:LEU:CD2	1:A:563:MET:HE2	2.31	0.56
1:G:362:LYS:HG3	1:G:371:TYR:CE1	2.39	0.56
1:A:653:ALA:HB2	1:A:742:VAL:HG21	1.87	0.56
1:A:655:GLY:O	1:A:656:TYR:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:GLU:HG3	1:A:581:TYR:HE1	1.70	0.56
1:E:182:ARG:O	1:G:598:ARG:HD3	2.06	0.56
1:I:93:ALA:HB2	1:I:167:PRO:HD2	1.88	0.56
2:N:18:ARG:HD3	1:O:624:ASP:OD2	2.05	0.56
1:O:183:THR:HG21	1:O:314:ASP:C	2.31	0.56
1:A:572:THR:HB	1:A:574:TRP:CD1	2.41	0.56
1:I:568:GLU:HG3	1:I:581:TYR:CE1	2.40	0.56
1:I:542:MET:HE1	1:I:750:LEU:N	2.21	0.56
1:A:362:LYS:HG3	1:A:371:TYR:CE1	2.40	0.56
1:A:394:LEU:HA	1:A:563:MET:CE	2.35	0.56
1:A:216:ILE:O	1:A:217:ALA:HB3	2.05	0.56
2:B:53:PHE:CZ	2:B:116:MET:HE1	2.40	0.56
1:G:542:MET:CE	1:G:750:LEU:HA	2.31	0.56
1:G:568:GLU:HG3	1:G:581:TYR:CE1	2.39	0.56
1:I:216:ILE:O	1:I:217:ALA:HB3	2.05	0.56
1:O:518:SER:HB3	1:O:730:LEU:HD12	1.87	0.56
1:O:542:MET:HE1	1:O:750:LEU:N	2.21	0.56
1:O:568:GLU:HG3	1:O:581:TYR:CE1	2.41	0.56
1:E:694:PRO:HA	1:E:698:MET:HE2	1.88	0.55
2:H:53:PHE:CZ	2:H:116:MET:HE1	2.40	0.55
1:A:688:PRO:HG2	1:C:688:PRO:CG	2.25	0.55
1:G:568:GLU:HG3	1:G:581:TYR:HE1	1.72	0.55
1:O:362:LYS:HG3	1:O:371:TYR:CE1	2.40	0.55
1:O:542:MET:HE2	1:O:749:VAL:CG1	2.25	0.55
2:J:18:ARG:HD3	1:K:624:ASP:OD2	2.06	0.55
1:A:183:THR:HG21	1:A:314:ASP:C	2.30	0.55
1:G:518:SER:HB3	1:G:730:LEU:HD12	1.88	0.55
1:G:542:MET:HE2	1:G:749:VAL:CG1	2.23	0.55
1:C:676:SER:HA	1:C:708:ALA:O	2.07	0.55
1:I:542:MET:HE2	1:I:749:VAL:CG1	2.25	0.55
1:M:609:SER:OG	1:M:705:PHE:O	2.24	0.55
1:M:688:PRO:HG2	1:O:688:PRO:CG	2.27	0.55
1:O:729:TRP:CE2	1:O:742:VAL:HG13	2.41	0.55
1:A:283:ILE:HG23	1:A:283:ILE:O	2.06	0.55
1:A:542:MET:HE1	1:A:750:LEU:N	2.22	0.55
1:O:568:GLU:HG3	1:O:581:TYR:HE1	1.72	0.55
1:A:302:ASN:HA	1:A:338:ASP:OD1	2.07	0.55
1:A:598:ARG:HG3	1:A:598:ARG:NH1	2.21	0.55
1:I:283:ILE:HG23	1:I:283:ILE:O	2.06	0.55
1:I:394:LEU:CD2	1:I:563:MET:HE2	2.31	0.55
1:G:183:THR:HG21	1:G:314:ASP:C	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:38:LEU:HD23	1:K:58:ILE:CG2	2.37	0.55
1:G:194:ASP:HB2	2:H:7:SER:N	2.21	0.55
1:K:676:SER:HA	1:K:708:ALA:O	2.07	0.55
1:G:572:THR:HB	1:G:574:TRP:CD1	2.43	0.54
1:M:216:ILE:O	1:M:217:ALA:HB3	2.07	0.54
1:C:88:LEU:HD13	1:C:214:LEU:HD13	1.87	0.54
1:C:183:THR:HG21	1:C:314:ASP:CA	2.38	0.54
1:E:216:ILE:O	1:E:217:ALA:HB3	2.07	0.54
1:I:729:TRP:HH2	1:I:745:MET:HE2	1.72	0.54
1:M:657:GLU:HG3	1:M:727:ILE:HD12	1.88	0.54
1:O:194:ASP:HB2	2:P:7:SER:N	2.22	0.54
1:A:518:SER:HB3	1:A:730:LEU:HD12	1.89	0.54
1:E:552:ILE:HD11	1:E:596:ARG:HG3	1.88	0.54
1:I:183:THR:HG21	1:I:314:ASP:C	2.31	0.54
1:I:598:ARG:HG3	1:I:598:ARG:NH1	2.21	0.54
1:I:653:ALA:HB2	1:I:742:VAL:HG21	1.89	0.54
1:K:687:ILE:HD12	5:K:911:HOH:O	2.05	0.54
1:O:572:THR:HB	1:O:574:TRP:CD1	2.43	0.54
1:A:134:VAL:HG22	1:A:148:VAL:HG22	1.88	0.54
1:G:394:LEU:HD22	1:G:563:MET:CE	2.29	0.54
1:G:653:ALA:HB2	1:G:742:VAL:HG21	1.89	0.54
1:I:394:LEU:HD22	1:I:563:MET:CE	2.30	0.54
1:I:572:THR:HB	1:I:574:TRP:CD1	2.43	0.54
1:K:694:PRO:HA	1:K:698:MET:HE2	1.89	0.54
1:A:729:TRP:CE2	1:A:742:VAL:HG13	2.43	0.54
1:O:542:MET:CE	1:O:750:LEU:HA	2.34	0.54
1:A:553:VAL:CG1	1:A:563:MET:HG3	2.37	0.54
1:C:632:TRP:CE2	1:C:760:PRO:HG2	2.43	0.54
1:K:594:ARG:NH1	5:K:903:HOH:O	2.40	0.54
1:O:216:ILE:O	1:O:217:ALA:HB3	2.06	0.54
1:O:394:LEU:CD2	1:O:563:MET:HE2	2.31	0.54
1:E:88:LEU:HD13	1:E:214:LEU:HD13	1.88	0.54
1:C:447:ARG:HD3	1:C:448:GLY:O	2.07	0.54
1:I:194:ASP:HB2	2:J:7:SER:N	2.23	0.54
1:I:611:PHE:HB3	1:I:657:GLU:HG3	1.90	0.54
1:I:729:TRP:CZ2	1:I:742:VAL:HG13	2.42	0.54
1:E:183:THR:HG21	1:E:314:ASP:CA	2.38	0.54
1:G:394:LEU:HA	1:G:563:MET:CE	2.38	0.54
1:K:216:ILE:O	1:K:217:ALA:HB3	2.07	0.54
1:K:294:TYR:HH	1:O:455:ARG:HH22	1.50	0.54
1:O:729:TRP:HH2	1:O:745:MET:HE2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:SER:HB2	1:A:331:TRP:HB3	1.89	0.54
1:A:729:TRP:CZ2	1:A:742:VAL:HG13	2.42	0.54
1:E:412:GLN:CB	2:F:78:ARG:HH22	2.13	0.54
1:G:302:ASN:HA	1:G:338:ASP:OD1	2.08	0.54
2:L:25:PHE:CZ	2:L:29:ARG:HD2	2.42	0.54
1:M:183:THR:HG21	1:M:314:ASP:CA	2.37	0.54
1:I:134:VAL:HG22	1:I:148:VAL:HG22	1.89	0.53
1:I:568:GLU:HG3	1:I:581:TYR:HE1	1.73	0.53
1:I:729:TRP:CE2	1:I:742:VAL:HG13	2.43	0.53
1:E:412:GLN:NE2	2:F:78:ARG:HH21	2.05	0.53
1:E:676:SER:HA	1:E:708:ALA:O	2.08	0.53
1:G:724:THR:HG21	1:G:729:TRP:CE2	2.43	0.53
1:C:159:TYR:HE1	1:C:195:SER:HB3	1.73	0.53
1:G:216:ILE:O	1:G:217:ALA:HB3	2.07	0.53
1:G:729:TRP:CZ2	1:G:742:VAL:HG13	2.44	0.53
2:H:72:MET:O	2:H:72:MET:HG3	2.08	0.53
2:F:18:ARG:HD3	1:G:624:ASP:OD2	2.07	0.53
1:I:578:PRO:HG2	1:K:597:ALA:HB2	1.90	0.53
2:F:51:ASN:HD21	2:F:55:TYR:N	2.06	0.53
1:G:598:ARG:HG3	1:G:598:ARG:NH1	2.21	0.53
1:I:12:ARG:CB	1:M:266:ILE:HD13	2.38	0.53
1:K:88:LEU:HD13	1:K:214:LEU:HD13	1.90	0.53
1:K:109:ARG:HG3	1:K:129:GLU:HG2	1.91	0.53
1:M:159:TYR:HE1	1:M:195:SER:HB3	1.74	0.53
1:O:134:VAL:HG22	1:O:148:VAL:HG22	1.90	0.53
1:E:643:ILE:HD13	1:E:745:MET:HE2	1.90	0.53
1:I:624:ASP:OD2	2:L:18:ARG:HD3	2.09	0.53
1:K:159:TYR:HE1	1:K:195:SER:HB3	1.74	0.53
1:M:624:ASP:OD2	2:P:18:ARG:HD3	2.09	0.53
1:M:643:ILE:HD13	1:M:745:MET:HE2	1.89	0.53
1:O:22:ARG:HD2	1:O:344:LYS:HD3	1.90	0.53
1:O:653:ALA:HB2	1:O:742:VAL:HG21	1.90	0.53
1:I:553:VAL:CG1	1:I:563:MET:HG3	2.39	0.53
2:J:53:PHE:CZ	2:J:116:MET:HE1	2.43	0.53
1:K:632:TRP:CE2	1:K:760:PRO:HG2	2.44	0.53
1:O:283:ILE:HG23	1:O:283:ILE:O	2.09	0.53
1:C:7:ARG:N	1:C:7:ARG:HD2	2.24	0.53
1:O:724:THR:HG21	1:O:729:TRP:CE2	2.43	0.53
1:G:134:VAL:HG22	1:G:148:VAL:HG22	1.91	0.53
1:I:302:ASN:HA	1:I:338:ASP:OD1	2.09	0.53
1:O:624:ASP:HB2	1:O:673:LEU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:PHE:HB3	1:A:657:GLU:HG3	1.91	0.52
1:E:183:THR:HG21	1:E:314:ASP:C	2.35	0.52
1:E:409:ASP:OD2	2:F:74:PRO:HA	2.09	0.52
1:G:729:TRP:CE2	1:G:742:VAL:HG13	2.44	0.52
1:K:570:GLY:HA3	1:K:574:TRP:CZ2	2.44	0.52
1:A:137:ILE:HD13	1:A:172:LEU:HD21	1.91	0.52
1:C:38:LEU:HD23	1:C:58:ILE:CG2	2.38	0.52
1:C:609:SER:HB3	1:C:658:LEU:O	2.09	0.52
1:I:62:LEU:HD12	1:I:62:LEU:C	2.34	0.52
1:I:624:ASP:HB2	1:I:673:LEU:O	2.09	0.52
1:K:148:VAL:O	1:K:199:VAL:HG21	2.09	0.52
1:K:643:ILE:HD13	1:K:745:MET:HE2	1.90	0.52
1:O:302:ASN:HA	1:O:338:ASP:OD1	2.08	0.52
2:H:28:GLU:OE2	2:H:32:LYS:HE3	2.10	0.52
1:K:7:ARG:HD2	1:K:7:ARG:N	2.25	0.52
1:E:447:ARG:HD3	1:E:448:GLY:O	2.08	0.52
1:E:519:HIS:CE1	1:E:547:ASN:HD22	2.27	0.52
2:F:53:PHE:CZ	2:F:116:MET:HE1	2.44	0.52
1:G:611:PHE:HB3	1:G:657:GLU:HG3	1.90	0.52
1:M:392:SER:HA	1:M:497:GLU:CD	2.35	0.52
1:C:109:ARG:HG3	1:C:129:GLU:HG2	1.91	0.52
1:G:283:ILE:HG23	1:G:283:ILE:O	2.08	0.52
1:K:447:ARG:HD3	1:K:448:GLY:O	2.09	0.52
1:C:394:LEU:CD2	1:C:563:MET:HE2	2.29	0.52
1:C:598:ARG:HH11	1:C:598:ARG:CG	2.12	0.52
1:G:62:LEU:C	1:G:62:LEU:HD12	2.35	0.52
1:I:394:LEU:HA	1:I:563:MET:CE	2.38	0.52
1:I:604:TRP:CD1	1:I:721:MET:HE2	2.45	0.52
1:K:394:LEU:CD2	1:K:563:MET:HE2	2.31	0.52
1:M:109:ARG:HG3	1:M:129:GLU:HG2	1.91	0.52
1:M:521:GLU:HA	1:M:547:ASN:O	2.10	0.52
1:O:519:HIS:CE1	1:O:547:ASN:HD22	2.27	0.52
1:O:598:ARG:HG3	1:O:598:ARG:NH1	2.21	0.52
1:A:703:HIS:CD2	2:D:72:MET:HE1	2.45	0.52
1:A:724:THR:HG21	1:A:729:TRP:CE2	2.44	0.52
1:A:604:TRP:CD1	1:A:721:MET:HE2	2.45	0.52
1:C:90:PRO:HG2	1:C:94:PHE:HB3	1.92	0.52
1:O:611:PHE:HB3	1:O:657:GLU:HG3	1.91	0.52
1:A:109:ARG:NH2	1:A:118:ASP:OD2	2.43	0.52
2:B:28:GLU:OE2	2:B:32:LYS:HE3	2.10	0.52
1:C:687:ILE:HD12	5:C:906:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:TYR:HE1	1:E:195:SER:HB3	1.75	0.52
1:C:394:LEU:HA	1:C:563:MET:CE	2.41	0.51
1:G:657:GLU:HB2	1:G:727:ILE:HD12	1.91	0.51
1:K:598:ARG:HH11	1:K:598:ARG:CG	2.13	0.51
1:O:475:LEU:HB3	1:O:476:PRO:HD3	1.91	0.51
2:P:28:GLU:OE2	2:P:32:LYS:HE3	2.10	0.51
1:G:519:HIS:CE1	1:G:547:ASN:HD22	2.27	0.51
1:I:518:SER:CB	1:I:730:LEU:HD12	2.41	0.51
1:M:183:THR:HG21	1:M:314:ASP:C	2.36	0.51
1:C:271:HIS:O	1:C:291:ALA:N	2.43	0.51
2:D:53:PHE:CZ	2:D:116:MET:HE1	2.46	0.51
1:E:101:TRP:HB3	1:E:238:LYS:HB2	1.93	0.51
1:G:553:VAL:HG22	1:G:565:VAL:HB	1.93	0.51
1:I:724:THR:HG21	1:I:729:TRP:CE2	2.45	0.51
2:L:30:ARG:O	2:L:34:ILE:HG12	2.11	0.51
1:M:632:TRP:CE2	1:M:760:PRO:HG2	2.45	0.51
1:A:62:LEU:HD12	1:A:62:LEU:C	2.35	0.51
1:C:103:THR:HG22	1:C:156:GLN:HG3	1.92	0.51
1:E:90:PRO:HG2	1:E:94:PHE:HB3	1.92	0.51
1:G:553:VAL:CG1	1:G:563:MET:HG3	2.38	0.51
1:I:519:HIS:CE1	1:I:547:ASN:HD22	2.26	0.51
1:M:148:VAL:O	1:M:199:VAL:HG21	2.11	0.51
1:A:542:MET:CE	1:A:750:LEU:HA	2.34	0.51
1:K:90:PRO:HG2	1:K:94:PHE:HB3	1.93	0.51
1:M:729:TRP:CE2	1:M:742:VAL:HG13	2.46	0.51
1:A:302:ASN:O	1:A:336:CYS:HB3	2.10	0.51
1:E:729:TRP:CE2	1:E:742:VAL:HG13	2.45	0.51
1:G:22:ARG:HD2	1:G:344:LYS:HD3	1.93	0.51
1:M:7:ARG:HD2	1:M:7:ARG:N	2.25	0.51
1:M:88:LEU:HD13	1:M:214:LEU:HD13	1.92	0.51
1:E:38:LEU:HD23	1:E:58:ILE:CG2	2.40	0.51
1:E:103:THR:HG22	1:E:156:GLN:HG3	1.93	0.51
1:G:302:ASN:O	1:G:336:CYS:HB3	2.10	0.51
1:I:388:LEU:HD13	1:I:511:TYR:CZ	2.46	0.51
1:K:519:HIS:CE1	1:K:521:GLU:HB2	2.45	0.51
1:O:305:SER:HB2	1:O:331:TRP:HB3	1.91	0.51
1:C:109:ARG:HG3	1:C:129:GLU:CG	2.41	0.51
1:E:521:GLU:HA	1:E:547:ASN:O	2.11	0.51
2:L:51:ASN:HD21	2:L:55:TYR:N	2.08	0.51
2:B:75:THR:O	2:B:78:ARG:HB2	2.09	0.51
1:C:570:GLY:HA3	1:C:574:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:ARG:O	2:D:34:ILE:HG12	2.11	0.51
1:E:412:GLN:HE22	2:F:123:ARG:HH22	1.58	0.51
1:E:570:GLY:HA3	1:E:574:TRP:CZ2	2.46	0.51
1:E:685:THR:HG22	1:E:686:VAL:N	2.26	0.51
1:G:109:ARG:NH2	1:G:118:ASP:OD2	2.43	0.51
1:G:394:LEU:CD2	1:G:563:MET:HE2	2.32	0.51
1:K:266:ILE:HD13	1:O:12:ARG:HB2	1.92	0.51
1:K:519:HIS:CE1	1:K:547:ASN:HD22	2.27	0.51
2:N:53:PHE:CZ	2:N:116:MET:HE1	2.45	0.51
1:C:685:THR:HG22	1:C:686:VAL:N	2.26	0.51
1:E:109:ARG:HG3	1:E:129:GLU:CG	2.40	0.51
2:J:130:GLU:O	2:J:131:LEU:HD23	2.11	0.51
1:K:151:ARG:HG2	1:K:195:SER:HA	1.92	0.51
1:M:394:LEU:HA	1:M:563:MET:CE	2.41	0.51
1:M:472:ILE:HD12	1:M:477:ALA:HA	1.93	0.51
1:E:409:ASP:O	2:F:78:ARG:NH1	2.44	0.50
1:G:388:LEU:HD13	1:G:511:TYR:CZ	2.46	0.50
1:G:402:GLU:HG2	1:G:404:ILE:HG13	1.93	0.50
1:I:481:LEU:HB2	1:I:730:LEU:HD22	1.94	0.50
2:J:49:ALA:HB2	2:J:117:HIS:CE1	2.46	0.50
2:L:53:PHE:CZ	2:L:116:MET:HE1	2.47	0.50
1:M:23:PHE:CB	1:M:346:PHE:CE1	2.94	0.50
1:M:402:GLU:HG2	1:M:404:ILE:H	1.76	0.50
1:O:553:VAL:HG22	1:O:565:VAL:HB	1.94	0.50
1:O:622:MET:HB3	1:O:623:PRO:CD	2.41	0.50
1:A:553:VAL:HG22	1:A:565:VAL:HB	1.92	0.50
1:E:624:ASP:OD2	2:H:18:ARG:HD3	2.11	0.50
1:E:632:TRP:CE2	1:E:760:PRO:HG2	2.46	0.50
1:E:638:ASP:OD2	1:O:756:ASP:O	2.29	0.50
1:M:447:ARG:HD3	1:M:448:GLY:O	2.09	0.50
1:C:729:TRP:CE2	1:C:742:VAL:HG13	2.46	0.50
2:D:51:ASN:HD21	2:D:55:TYR:N	2.09	0.50
1:K:109:ARG:HG3	1:K:129:GLU:CG	2.41	0.50
1:K:685:THR:HG22	1:K:686:VAL:N	2.26	0.50
2:N:51:ASN:HD21	2:N:55:TYR:N	2.09	0.50
1:O:62:LEU:C	1:O:62:LEU:HD12	2.36	0.50
1:A:22:ARG:HD2	1:A:344:LYS:HD3	1.92	0.50
1:E:578:PRO:HG2	1:G:597:ALA:HB2	1.92	0.50
1:I:302:ASN:O	1:I:336:CYS:HB3	2.11	0.50
1:K:392:SER:HA	1:K:497:GLU:CD	2.37	0.50
1:M:346:PHE:CD1	1:M:346:PHE:C	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:VAL:O	1:E:199:VAL:HG21	2.11	0.50
1:E:151:ARG:HG2	1:E:195:SER:HA	1.94	0.50
1:M:519:HIS:CE1	1:M:547:ASN:HD22	2.29	0.50
2:P:38:ILE:HD13	2:P:44:ILE:HD11	1.93	0.50
1:A:475:LEU:HB3	1:A:476:PRO:HD3	1.93	0.50
1:O:657:GLU:HB2	1:O:727:ILE:HD12	1.93	0.50
2:B:130:GLU:O	2:B:131:LEU:HD23	2.12	0.50
1:C:519:HIS:CE1	1:C:547:ASN:HD22	2.28	0.50
1:M:687:ILE:HD12	5:M:902:HOH:O	2.12	0.50
1:C:101:TRP:HB3	1:C:238:LYS:HB2	1.93	0.50
1:C:183:THR:HG21	1:C:314:ASP:C	2.37	0.50
1:G:475:LEU:HB3	1:G:476:PRO:HD3	1.92	0.50
1:I:22:ARG:HD2	1:I:344:LYS:HD3	1.92	0.50
2:J:38:ILE:HD13	2:J:44:ILE:HD11	1.94	0.50
1:K:609:SER:HB3	1:K:658:LEU:O	2.11	0.50
1:M:570:GLY:HA3	1:M:574:TRP:CZ2	2.47	0.50
1:O:553:VAL:CG1	1:O:563:MET:HG3	2.40	0.50
1:G:305:SER:HB2	1:G:331:TRP:HB3	1.92	0.50
1:I:305:SER:HB2	1:I:331:TRP:HB3	1.94	0.50
1:M:109:ARG:HG3	1:M:129:GLU:CG	2.41	0.50
1:M:609:SER:HB3	1:M:658:LEU:O	2.11	0.50
2:N:30:ARG:O	2:N:34:ILE:HG12	2.11	0.50
1:O:447:ARG:HD3	1:O:448:GLY:O	2.12	0.50
1:C:151:ARG:HG2	1:C:195:SER:HA	1.92	0.49
1:G:165:TYR:CE2	1:G:167:PRO:HG3	2.47	0.49
1:G:601:GLN:HG3	1:G:606:THR:HA	1.94	0.49
1:I:137:ILE:HD13	1:I:172:LEU:HD21	1.93	0.49
1:I:521:GLU:HA	1:I:547:ASN:O	2.12	0.49
2:P:130:GLU:O	2:P:131:LEU:HD23	2.12	0.49
1:A:147:VAL:HG22	1:A:199:VAL:HG23	1.94	0.49
1:E:472:ILE:HD12	1:E:477:ALA:HA	1.94	0.49
1:I:5:ALA:HB3	1:I:368:THR:HG21	1.94	0.49
1:I:109:ARG:NH2	1:I:118:ASP:OD2	2.45	0.49
1:K:62:LEU:HD12	1:K:62:LEU:C	2.38	0.49
1:M:90:PRO:HG2	1:M:94:PHE:HB3	1.93	0.49
1:A:518:SER:CB	1:A:730:LEU:HD12	2.42	0.49
1:G:604:TRP:CD1	1:G:721:MET:HE2	2.47	0.49
1:I:147:VAL:HG22	1:I:199:VAL:HG23	1.95	0.49
1:K:183:THR:HG21	1:K:314:ASP:C	2.36	0.49
1:K:729:TRP:CE2	1:K:742:VAL:HG13	2.47	0.49
1:A:622:MET:HB3	1:A:623:PRO:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:VAL:HG22	1:G:199:VAL:HG23	1.94	0.49
1:K:412:GLN:HG2	2:L:71:ARG:HG2	1.94	0.49
1:A:447:ARG:HD3	1:A:448:GLY:O	2.12	0.49
1:E:400:ALA:O	1:E:438:SER:HB3	2.12	0.49
1:E:632:TRP:CD1	1:E:632:TRP:H	2.31	0.49
1:I:11:ASP:OD2	1:I:22:ARG:NH1	2.46	0.49
1:I:12:ARG:HB3	1:M:266:ILE:HD13	1.94	0.49
1:I:165:TYR:CE2	1:I:167:PRO:HG3	2.47	0.49
1:I:553:VAL:HG22	1:I:565:VAL:HB	1.93	0.49
1:I:622:MET:HB3	1:I:623:PRO:CD	2.43	0.49
1:K:553:VAL:HG13	1:K:563:MET:HG3	1.94	0.49
2:N:72:MET:HE1	1:O:703:HIS:CD2	2.47	0.49
1:E:7:ARG:N	1:E:7:ARG:HD2	2.27	0.49
1:M:685:THR:HG22	1:M:686:VAL:N	2.28	0.49
1:O:518:SER:CB	1:O:730:LEU:HD12	2.41	0.49
1:C:214:LEU:HD23	1:C:214:LEU:C	2.38	0.49
1:G:518:SER:CB	1:G:730:LEU:HD12	2.42	0.49
1:I:402:GLU:HG2	1:I:404:ILE:HG13	1.94	0.49
1:K:271:HIS:O	1:K:291:ALA:N	2.44	0.49
1:M:38:LEU:HD23	1:M:58:ILE:CG2	2.43	0.49
1:M:151:ARG:HG2	1:M:195:SER:HA	1.94	0.49
1:O:394:LEU:HA	1:O:563:MET:CE	2.38	0.49
1:A:694:PRO:HA	1:A:698:MET:HE2	1.95	0.49
1:C:394:LEU:C	1:C:563:MET:HE1	2.38	0.49
1:C:521:GLU:HA	1:C:547:ASN:O	2.13	0.49
2:F:30:ARG:O	2:F:34:ILE:HG12	2.12	0.49
1:K:394:LEU:HA	1:K:563:MET:CE	2.43	0.49
1:O:147:VAL:HG22	1:O:199:VAL:HG23	1.94	0.49
1:O:402:GLU:HG2	1:O:404:ILE:HG13	1.95	0.49
1:A:519:HIS:CE1	1:A:521:GLU:HB2	2.48	0.49
1:E:542:MET:CE	1:E:749:VAL:HG12	2.36	0.49
1:E:609:SER:HB3	1:E:658:LEU:O	2.11	0.49
1:K:394:LEU:C	1:K:563:MET:HE1	2.38	0.49
1:C:338:ASP:HA	1:C:453:SER:HB2	1.95	0.49
1:M:62:LEU:C	1:M:62:LEU:HD12	2.38	0.49
1:E:392:SER:HA	1:E:497:GLU:CD	2.38	0.48
1:M:103:THR:HG22	1:M:156:GLN:HG3	1.95	0.48
1:M:346:PHE:C	1:M:346:PHE:HD1	2.21	0.48
1:M:632:TRP:H	1:M:632:TRP:CD1	2.30	0.48
1:O:302:ASN:O	1:O:336:CYS:HB3	2.13	0.48
1:C:400:ALA:O	1:C:438:SER:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:694:PRO:HA	1:G:698:MET:HE2	1.95	0.48
1:M:410:ILE:HD11	1:O:693:PHE:HB3	1.95	0.48
2:N:33:GLU:O	2:N:37:ILE:HG13	2.13	0.48
1:O:109:ARG:NH2	1:O:118:ASP:OD2	2.45	0.48
1:O:521:GLU:HA	1:O:547:ASN:O	2.13	0.48
1:C:148:VAL:O	1:C:199:VAL:HG21	2.13	0.48
1:G:101:TRP:HB3	1:G:238:LYS:HB2	1.96	0.48
1:I:475:LEU:HB3	1:I:476:PRO:HD3	1.94	0.48
1:M:183:THR:HG23	1:M:313:TRP:O	2.13	0.48
1:O:542:MET:CE	1:O:749:VAL:HG12	2.26	0.48
1:A:521:GLU:HA	1:A:547:ASN:O	2.14	0.48
1:A:601:GLN:HG3	1:A:606:THR:HA	1.95	0.48
1:E:306:ARG:HG2	1:E:330:LEU:CD2	2.43	0.48
1:E:394:LEU:HA	1:E:563:MET:CE	2.43	0.48
1:G:137:ILE:HD13	1:G:172:LEU:HD21	1.94	0.48
1:O:601:GLN:HG3	1:O:606:THR:HA	1.94	0.48
1:E:214:LEU:C	1:E:214:LEU:HD23	2.39	0.48
1:K:519:HIS:HE1	1:K:547:ASN:ND2	2.11	0.48
1:O:90:PRO:HG2	1:O:94:PHE:HB3	1.95	0.48
1:C:632:TRP:CD1	1:C:632:TRP:H	2.32	0.48
1:E:519:HIS:CE1	1:E:521:GLU:HB2	2.49	0.48
1:G:521:GLU:HA	1:G:547:ASN:O	2.14	0.48
1:K:472:ILE:HD12	1:K:477:ALA:HA	1.94	0.48
1:K:521:GLU:HA	1:K:547:ASN:O	2.14	0.48
1:O:388:LEU:HD13	1:O:511:TYR:CZ	2.49	0.48
1:O:604:TRP:CD1	1:O:721:MET:HE2	2.48	0.48
1:A:5:ALA:HB3	1:A:368:THR:HG21	1.95	0.48
1:A:388:LEU:HD13	1:A:511:TYR:CZ	2.48	0.48
1:A:624:ASP:HB2	1:A:673:LEU:O	2.14	0.48
1:E:622:MET:O	1:E:625:SER:HB2	2.13	0.48
1:K:632:TRP:H	1:K:632:TRP:CD1	2.30	0.48
1:M:101:TRP:HB3	1:M:238:LYS:HB2	1.96	0.48
1:M:394:LEU:C	1:M:563:MET:HE1	2.38	0.48
1:O:165:TYR:CE2	1:O:167:PRO:HG3	2.49	0.48
1:A:11:ASP:OD2	1:A:22:ARG:NH1	2.47	0.48
1:G:481:LEU:HB2	1:G:730:LEU:HD22	1.96	0.48
1:I:90:PRO:HG2	1:I:94:PHE:HB3	1.96	0.48
1:K:101:TRP:HB3	1:K:238:LYS:HB2	1.95	0.48
1:M:519:HIS:CE1	1:M:521:GLU:HB2	2.49	0.48
1:A:628:GLU:H	1:A:628:GLU:HG3	1.37	0.48
1:C:62:LEU:C	1:C:62:LEU:HD12	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:HIS:CE1	1:C:521:GLU:HB2	2.49	0.48
2:J:28:GLU:OE2	2:J:32:LYS:HE3	2.14	0.48
1:K:338:ASP:HA	1:K:453:SER:HB2	1.96	0.48
1:M:214:LEU:HD23	1:M:214:LEU:C	2.39	0.48
1:O:101:TRP:HB3	1:O:238:LYS:HB2	1.96	0.48
1:E:402:GLU:HG2	1:E:404:ILE:H	1.79	0.48
1:O:481:LEU:HB2	1:O:730:LEU:HD22	1.96	0.48
1:G:622:MET:HB3	1:G:623:PRO:CD	2.43	0.47
2:H:130:GLU:O	2:H:131:LEU:HD23	2.14	0.47
1:K:101:TRP:CH2	1:K:156:GLN:HG2	2.49	0.47
1:C:168:GLU:HA	1:C:168:GLU:OE1	2.14	0.47
1:G:624:ASP:HB2	1:G:673:LEU:O	2.14	0.47
1:K:622:MET:O	1:K:625:SER:HB2	2.13	0.47
1:A:165:TYR:CE2	1:A:167:PRO:HG3	2.48	0.47
1:A:190:VAL:HG21	1:C:602:LYS:O	2.13	0.47
1:A:467:GLN:OE1	1:A:469:PHE:HB2	2.15	0.47
1:C:472:ILE:HD12	1:C:477:ALA:HA	1.95	0.47
1:C:519:HIS:HE1	1:C:547:ASN:ND2	2.12	0.47
1:C:643:ILE:HG21	1:C:745:MET:CE	2.43	0.47
1:G:402:GLU:HG2	1:G:404:ILE:H	1.79	0.47
1:I:601:GLN:HG3	1:I:606:THR:HA	1.96	0.47
1:K:38:LEU:HD23	1:K:58:ILE:HG21	1.96	0.47
1:M:400:ALA:O	1:M:438:SER:HB3	2.13	0.47
2:P:25:PHE:CZ	2:P:29:ARG:HD2	2.50	0.47
1:C:542:MET:HE1	1:C:750:LEU:N	2.29	0.47
1:E:394:LEU:C	1:E:563:MET:HE1	2.40	0.47
1:E:597:ALA:HB2	1:G:578:PRO:HG2	1.96	0.47
1:G:5:ALA:HA	1:G:28:ASN:HD21	1.80	0.47
1:G:447:ARG:HD3	1:G:448:GLY:O	2.15	0.47
2:H:25:PHE:CZ	2:H:29:ARG:HD2	2.50	0.47
1:M:622:MET:O	1:M:625:SER:HB2	2.15	0.47
1:A:572:THR:HB	1:A:574:TRP:HD1	1.78	0.47
1:A:693:PHE:HB3	1:C:410:ILE:HD11	1.96	0.47
1:C:101:TRP:CH2	1:C:156:GLN:HG2	2.50	0.47
1:E:236:ASN:HB3	1:E:445:ASP:OD1	2.15	0.47
2:F:71:ARG:O	2:F:78:ARG:NH2	2.47	0.47
1:K:542:MET:HE1	1:K:750:LEU:N	2.29	0.47
1:A:519:HIS:CE1	1:A:547:ASN:HD22	2.29	0.47
1:E:402:GLU:CG	1:E:404:ILE:HG13	2.44	0.47
1:I:447:ARG:HD3	1:I:448:GLY:O	2.14	0.47
2:J:72:MET:HE2	2:J:72:MET:HB2	1.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:103:THR:HG22	1:K:156:GLN:HG3	1.96	0.47
1:K:421:LEU:HD12	2:L:80:TYR:CD2	2.50	0.47
1:O:166:ASP:OD2	1:O:169:LYS:HE3	2.15	0.47
1:C:392:SER:HA	1:C:497:GLU:CD	2.40	0.47
1:C:393:THR:HA	1:C:396:TYR:CD2	2.49	0.47
1:E:643:ILE:HG21	1:E:745:MET:CE	2.44	0.47
1:G:11:ASP:OD2	1:G:22:ARG:NH1	2.48	0.47
1:G:467:GLN:OE1	1:G:469:PHE:HB2	2.14	0.47
1:G:519:HIS:CE1	1:G:521:GLU:HB2	2.50	0.47
1:I:402:GLU:HG2	1:I:404:ILE:H	1.80	0.47
1:M:421:LEU:HD12	2:N:80:TYR:CD2	2.50	0.47
1:O:137:ILE:HD13	1:O:172:LEU:HD21	1.94	0.47
1:O:169:LYS:HB2	1:O:171:GLN:HB3	1.97	0.47
1:G:2:LYS:HB3	5:H:301:HOH:O	2.14	0.47
1:K:542:MET:CE	1:K:749:VAL:HG12	2.39	0.47
1:E:62:LEU:C	1:E:62:LEU:HD12	2.39	0.47
1:E:393:THR:HA	1:E:396:TYR:CD2	2.50	0.47
1:I:533:ASP:CG	1:K:182:ARG:HH22	2.23	0.47
1:O:467:GLN:OE1	1:O:469:PHE:HB2	2.15	0.47
1:G:365:TYR:O	1:G:368:THR:HG22	2.15	0.47
2:H:38:ILE:HD13	2:H:44:ILE:HD11	1.96	0.47
1:I:183:THR:HG21	1:I:314:ASP:HA	1.97	0.47
1:I:519:HIS:CE1	1:I:521:GLU:HB2	2.50	0.47
2:J:49:ALA:HB2	2:J:117:HIS:NE2	2.29	0.47
1:K:183:THR:HG23	1:K:313:TRP:O	2.15	0.47
1:E:109:ARG:HD2	1:E:129:GLU:OE2	2.15	0.46
1:E:516:THR:CG2	1:E:520:PRO:HG3	2.45	0.46
1:E:604:TRP:CD1	1:E:721:MET:HE2	2.51	0.46
1:G:90:PRO:HG2	1:G:94:PHE:HB3	1.97	0.46
1:K:393:THR:HA	1:K:396:TYR:CD2	2.50	0.46
1:A:182:ARG:HD3	1:C:598:ARG:NH2	2.30	0.46
1:C:306:ARG:HG2	1:C:330:LEU:CD2	2.45	0.46
1:C:474:GLU:OE1	1:C:474:GLU:HA	2.15	0.46
1:C:516:THR:CG2	1:C:520:PRO:HG3	2.46	0.46
1:E:519:HIS:HE1	1:E:547:ASN:ND2	2.12	0.46
1:I:472:ILE:CD1	1:I:477:ALA:HA	2.45	0.46
1:I:572:THR:HB	1:I:574:TRP:HD1	1.79	0.46
1:M:271:HIS:O	1:M:291:ALA:N	2.43	0.46
1:M:598:ARG:HH11	1:M:598:ARG:CG	2.13	0.46
1:O:283:ILE:O	5:O:901:HOH:O	2.21	0.46
1:O:519:HIS:CE1	1:O:521:GLU:HB2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ARG:HD3	1:C:624:ASP:OD2	2.14	0.46
1:C:183:THR:HG23	1:C:313:TRP:O	2.15	0.46
1:E:338:ASP:HA	1:E:453:SER:HB2	1.97	0.46
1:G:89:GLN:O	1:G:89:GLN:HG3	2.15	0.46
1:K:266:ILE:HD13	1:O:12:ARG:HB3	1.98	0.46
1:O:394:LEU:CB	1:O:563:MET:HE1	2.46	0.46
1:O:402:GLU:HG2	1:O:404:ILE:H	1.80	0.46
2:D:33:GLU:O	2:D:37:ILE:HG13	2.15	0.46
1:E:101:TRP:CH2	1:E:156:GLN:HG2	2.50	0.46
1:E:168:GLU:OE1	1:E:168:GLU:HA	2.15	0.46
1:G:5:ALA:HB3	1:G:368:THR:HG21	1.97	0.46
2:H:124:ILE:O	2:H:127:VAL:HG13	2.16	0.46
1:K:402:GLU:HG2	1:K:404:ILE:H	1.79	0.46
2:B:53:PHE:CE1	2:B:116:MET:HE1	2.50	0.46
1:C:622:MET:O	1:C:625:SER:HB2	2.15	0.46
1:E:271:HIS:O	1:E:291:ALA:N	2.44	0.46
1:G:371:TYR:O	1:G:373:PRO:HD3	2.15	0.46
1:M:338:ASP:HA	1:M:453:SER:HB2	1.96	0.46
1:A:90:PRO:HG2	1:A:94:PHE:HB3	1.97	0.46
1:A:125:ASN:HB2	1:A:219:LEU:CD2	2.46	0.46
1:A:657:GLU:HB2	1:A:727:ILE:HD12	1.97	0.46
1:I:657:GLU:HB2	1:I:727:ILE:HD12	1.97	0.46
1:K:168:GLU:HA	1:K:168:GLU:OE1	2.16	0.46
1:M:393:THR:HA	1:M:396:TYR:CD2	2.50	0.46
1:A:409:ASP:OD1	2:B:74:PRO:HA	2.16	0.46
2:D:104:LEU:HD12	2:D:104:LEU:HA	1.81	0.46
1:E:182:ARG:HH22	1:G:533:ASP:CG	2.22	0.46
1:E:412:GLN:NE2	2:F:78:ARG:NH2	2.63	0.46
1:M:604:TRP:CD1	1:M:721:MET:HE2	2.51	0.46
1:A:183:THR:HG21	1:A:314:ASP:HA	1.97	0.46
1:A:481:LEU:HB2	1:A:730:LEU:HD22	1.98	0.46
1:E:412:GLN:HG2	2:F:71:ARG:HG2	1.98	0.46
1:K:109:ARG:HD2	1:K:129:GLU:OE2	2.16	0.46
1:O:183:THR:HG21	1:O:314:ASP:HA	1.98	0.46
1:O:694:PRO:HA	1:O:698:MET:HE2	1.98	0.46
2:B:72:MET:HE1	1:C:703:HIS:CD2	2.51	0.46
1:C:532:GLU:HB2	1:C:603:ILE:CD1	2.46	0.46
1:E:183:THR:HG23	1:E:313:TRP:O	2.16	0.46
1:E:346:PHE:CD1	1:E:346:PHE:N	2.83	0.46
1:G:598:ARG:HH11	1:G:598:ARG:CG	2.29	0.46
1:K:384:THR:OG1	1:K:493:ASP:OD1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:101:TRP:CH2	1:M:156:GLN:HG2	2.50	0.46
1:M:306:ARG:HG2	1:M:330:LEU:CD2	2.46	0.46
2:P:49:ALA:HB2	2:P:117:HIS:NE2	2.31	0.46
2:P:53:PHE:CE1	2:P:116:MET:HE1	2.50	0.46
1:A:101:TRP:HB3	1:A:238:LYS:HB2	1.98	0.46
1:A:371:TYR:O	1:A:373:PRO:HD3	2.16	0.46
1:A:553:VAL:HG13	1:A:563:MET:CG	2.45	0.46
2:B:38:ILE:HD13	2:B:44:ILE:HD11	1.97	0.46
1:E:458:ILE:O	1:E:462:ARG:NH1	2.48	0.46
1:I:365:TYR:O	1:I:368:THR:HG22	2.16	0.46
1:I:467:GLN:OE1	1:I:469:PHE:HB2	2.17	0.46
1:I:598:ARG:HH11	1:I:598:ARG:CG	2.29	0.46
1:M:516:THR:CG2	1:M:520:PRO:HG3	2.46	0.46
1:M:553:VAL:HG13	1:M:563:MET:HG3	1.98	0.46
2:P:49:ALA:HB2	2:P:117:HIS:CE1	2.51	0.46
1:C:38:LEU:HD23	1:C:58:ILE:HG21	1.98	0.45
1:C:266:ILE:HD13	1:G:12:ARG:CB	2.46	0.45
1:C:505:ALA:O	1:C:509:ARG:HG3	2.16	0.45
1:E:100:LEU:HG	1:E:161:ILE:HD13	1.98	0.45
1:M:236:ASN:HB3	1:M:445:ASP:OD1	2.17	0.45
2:B:107:GLU:HG3	2:B:109:PHE:CZ	2.51	0.45
2:F:33:GLU:O	2:F:37:ILE:HG13	2.16	0.45
2:H:53:PHE:CE1	2:H:116:MET:HE1	2.51	0.45
1:O:89:GLN:O	1:O:89:GLN:HG3	2.16	0.45
1:M:384:THR:OG1	1:M:493:ASP:OD1	2.33	0.45
1:O:572:THR:HB	1:O:574:TRP:HD1	1.80	0.45
1:A:402:GLU:HG2	1:A:404:ILE:H	1.82	0.45
1:G:394:LEU:O	1:G:563:MET:HE1	2.17	0.45
1:I:596:ARG:NE	1:K:318:GLU:OE2	2.49	0.45
2:L:33:GLU:O	2:L:37:ILE:HG13	2.17	0.45
2:N:35:ILE:HD11	2:N:127:VAL:CG1	2.45	0.45
2:N:78:ARG:HD3	2:N:123:ARG:NH2	2.32	0.45
1:A:394:LEU:O	1:A:563:MET:HE1	2.17	0.45
1:A:402:GLU:HG2	1:A:404:ILE:HG13	1.97	0.45
1:E:598:ARG:HH11	1:E:598:ARG:CG	2.12	0.45
1:I:147:VAL:CG2	1:I:199:VAL:HG23	2.47	0.45
1:M:542:MET:HE1	1:M:750:LEU:N	2.31	0.45
1:M:678:VAL:O	1:M:679:GLU:HB2	2.15	0.45
1:O:11:ASP:OD2	1:O:22:ARG:NH1	2.50	0.45
1:O:394:LEU:CD2	1:O:563:MET:CE	2.93	0.45
1:C:402:GLU:CG	1:C:404:ILE:HG13	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:101:TRP:HB3	1:I:238:LYS:HB2	1.99	0.45
2:J:25:PHE:CZ	2:J:29:ARG:HD2	2.52	0.45
1:K:160:SER:C	1:K:161:ILE:HD12	2.41	0.45
1:K:458:ILE:O	1:K:462:ARG:NH1	2.49	0.45
1:M:62:LEU:HD23	1:M:348:PHE:CD1	2.51	0.45
1:M:160:SER:C	1:M:161:ILE:HD12	2.41	0.45
1:M:643:ILE:HG21	1:M:745:MET:CE	2.47	0.45
1:O:609:SER:HB3	1:O:658:LEU:O	2.16	0.45
1:E:74:GLN:HB2	1:E:230:TRP:CZ3	2.52	0.45
1:E:638:ASP:CG	1:O:756:ASP:O	2.59	0.45
1:G:570:GLY:HA3	1:G:574:TRP:CZ2	2.52	0.45
1:A:4:ILE:HB	1:A:427:GLU:CG	2.44	0.45
1:A:365:TYR:O	1:A:368:THR:HG22	2.17	0.45
1:E:62:LEU:HD23	1:E:348:PHE:CD1	2.51	0.45
2:H:49:ALA:HB2	2:H:117:HIS:CE1	2.52	0.45
1:I:475:LEU:C	1:I:475:LEU:HD23	2.41	0.45
1:I:694:PRO:HA	1:I:698:MET:HE2	1.99	0.45
1:K:643:ILE:HG21	1:K:745:MET:CE	2.46	0.45
1:O:371:TYR:O	1:O:373:PRO:HD3	2.16	0.45
1:A:147:VAL:CG2	1:A:199:VAL:HG23	2.47	0.45
1:A:598:ARG:HH11	1:A:598:ARG:CG	2.30	0.45
1:A:688:PRO:CG	1:C:688:PRO:HG2	2.28	0.45
1:K:40:ARG:NH2	1:K:42:ILE:HD11	2.32	0.45
1:M:74:GLN:HB2	1:M:230:TRP:CZ3	2.52	0.45
1:O:5:ALA:HB3	1:O:368:THR:HG21	1.99	0.45
1:O:365:TYR:O	1:O:368:THR:HG22	2.17	0.45
2:B:25:PHE:CZ	2:B:29:ARG:HD2	2.52	0.45
1:C:458:ILE:O	1:C:462:ARG:NH1	2.49	0.45
1:E:100:LEU:C	1:E:100:LEU:HD12	2.41	0.45
1:K:187:PHE:CD1	1:K:191:VAL:HG11	2.52	0.45
1:K:713:PHE:CZ	1:K:721:MET:HB3	2.52	0.45
1:C:100:LEU:HD12	1:C:100:LEU:C	2.42	0.44
1:C:553:VAL:HG13	1:C:563:MET:HG3	1.98	0.44
1:E:542:MET:HE1	1:E:750:LEU:N	2.31	0.44
1:G:553:VAL:HG13	1:G:563:MET:CG	2.45	0.44
1:I:4:ILE:HB	1:I:427:GLU:CG	2.44	0.44
1:I:183:THR:CG2	1:I:314:ASP:HA	2.47	0.44
1:I:214:LEU:HD11	1:I:244:ILE:HD11	1.99	0.44
1:I:628:GLU:H	1:I:628:GLU:HG3	1.38	0.44
1:O:331:TRP:CH2	1:O:447:ARG:HG3	2.52	0.44
1:A:331:TRP:CH2	1:A:447:ARG:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:519:HIS:HE1	1:G:547:ASN:ND2	2.15	0.44
1:K:402:GLU:CG	1:K:404:ILE:HG13	2.47	0.44
1:K:516:THR:CG2	1:K:520:PRO:HG3	2.47	0.44
1:M:23:PHE:CG	1:M:346:PHE:HE1	2.35	0.44
2:B:124:ILE:O	2:B:127:VAL:HG13	2.18	0.44
1:C:654:GLY:HA2	1:C:726:SER:OG	2.18	0.44
1:E:394:LEU:CD2	1:E:563:MET:HE2	2.34	0.44
1:E:691:LYS:NZ	1:G:575:GLU:HG2	2.33	0.44
1:G:472:ILE:CD1	1:G:477:ALA:HA	2.47	0.44
1:I:331:TRP:CH2	1:I:447:ARG:HG3	2.52	0.44
1:I:473:TRP:CE3	1:I:473:TRP:HA	2.52	0.44
1:M:168:GLU:HA	1:M:168:GLU:OE1	2.17	0.44
1:M:519:HIS:HE1	1:M:547:ASN:ND2	2.13	0.44
1:M:713:PHE:CZ	1:M:721:MET:HB3	2.52	0.44
1:O:472:ILE:CD1	1:O:477:ALA:HA	2.47	0.44
1:A:214:LEU:HD11	1:A:244:ILE:HD11	2.00	0.44
1:G:43:HIS:CE1	1:G:51:PRO:HG2	2.53	0.44
2:H:49:ALA:HB2	2:H:117:HIS:NE2	2.32	0.44
1:K:214:LEU:C	1:K:214:LEU:HD23	2.43	0.44
1:C:412:GLN:HG2	2:D:71:ARG:HG2	2.00	0.44
2:D:72:MET:HE3	2:D:72:MET:HB2	1.91	0.44
1:E:421:LEU:HD12	2:F:80:TYR:CD2	2.52	0.44
1:E:506:GLU:CG	1:I:756:ASP:CB	2.89	0.44
2:F:35:ILE:HD11	2:F:127:VAL:CG1	2.46	0.44
1:G:183:THR:HG21	1:G:314:ASP:HA	1.99	0.44
1:G:214:LEU:HD11	1:G:244:ILE:HD11	1.99	0.44
1:G:572:THR:HB	1:G:574:TRP:HD1	1.79	0.44
1:O:553:VAL:HG13	1:O:563:MET:CG	2.46	0.44
1:A:5:ALA:HA	1:A:28:ASN:HD21	1.82	0.44
1:A:570:GLY:HA3	1:A:574:TRP:CZ2	2.53	0.44
1:A:575:GLU:HG2	1:C:691:LYS:NZ	2.32	0.44
1:A:609:SER:HB3	1:A:658:LEU:O	2.17	0.44
1:E:564:GLU:OE1	1:E:585:THR:HG23	2.17	0.44
1:I:394:LEU:O	1:I:563:MET:HE1	2.18	0.44
1:K:346:PHE:N	1:K:346:PHE:CD1	2.82	0.44
1:M:377:LEU:HB3	1:M:378:PRO:HD2	1.98	0.44
1:A:183:THR:CG2	1:A:314:ASP:HA	2.48	0.44
1:C:40:ARG:NH2	1:C:42:ILE:HD11	2.33	0.44
1:C:365:TYR:O	1:C:366:GLU:HB2	2.17	0.44
1:C:713:PHE:CZ	1:C:721:MET:HB3	2.52	0.44
1:G:147:VAL:CG2	1:G:199:VAL:HG23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:700:GLY:HA2	1:G:706:VAL:HG11	2.00	0.44
1:K:508:LEU:HD22	1:K:514:VAL:HG21	1.99	0.44
1:K:532:GLU:HB2	1:K:603:ILE:CD1	2.48	0.44
1:M:100:LEU:HG	1:M:161:ILE:HD13	2.00	0.44
1:O:214:LEU:HD11	1:O:244:ILE:HD11	1.99	0.44
1:C:421:LEU:HD12	2:D:80:TYR:CD2	2.53	0.44
2:J:47:GLU:OE1	2:J:60:SER:HB3	2.18	0.44
1:K:91:ASP:OD1	1:K:91:ASP:N	2.26	0.44
1:M:508:LEU:HD22	1:M:514:VAL:HG21	1.99	0.44
1:C:109:ARG:HD2	1:C:129:GLU:OE2	2.18	0.44
1:C:518:SER:HB3	1:C:730:LEU:HD12	1.99	0.44
1:E:532:GLU:HB2	1:E:603:ILE:CD1	2.48	0.44
1:I:484:TRP:CG	1:I:733:LEU:HD13	2.53	0.44
1:I:519:HIS:HE1	1:I:547:ASN:ND2	2.13	0.44
1:K:100:LEU:HD12	1:K:100:LEU:C	2.43	0.44
1:M:109:ARG:HD2	1:M:129:GLU:OE2	2.17	0.44
1:A:569:LEU:HG	1:C:693:PHE:HD2	1.83	0.43
2:B:47:GLU:OE1	2:B:60:SER:HB3	2.18	0.43
1:E:518:SER:HB3	1:E:730:LEU:HD12	1.99	0.43
1:K:400:ALA:O	1:K:438:SER:HB3	2.18	0.43
1:K:516:THR:HG21	1:K:520:PRO:HG3	2.00	0.43
1:K:678:VAL:O	1:K:679:GLU:HB2	2.18	0.43
1:M:602:LYS:O	1:O:190:VAL:HG21	2.17	0.43
1:O:183:THR:CG2	1:O:314:ASP:HA	2.48	0.43
1:O:598:ARG:HH11	1:O:598:ARG:CG	2.31	0.43
1:A:484:TRP:CG	1:A:733:LEU:HD13	2.53	0.43
1:A:693:PHE:HB3	1:C:410:ILE:CD1	2.48	0.43
1:A:700:GLY:HA2	1:A:706:VAL:HG11	1.99	0.43
1:C:542:MET:CE	1:C:749:VAL:HG12	2.37	0.43
1:C:564:GLU:OE1	1:C:585:THR:HG23	2.18	0.43
1:E:9:TYR:CE2	1:E:340:CYS:HB2	2.53	0.43
1:E:90:PRO:HG2	1:E:94:PHE:CB	2.49	0.43
1:C:516:THR:HG21	1:C:520:PRO:HG3	2.01	0.43
1:E:553:VAL:HG13	1:E:563:MET:HG3	1.99	0.43
1:G:484:TRP:CG	1:G:733:LEU:HD13	2.53	0.43
1:G:657:GLU:HB2	1:G:727:ILE:CD1	2.49	0.43
2:H:107:GLU:HG3	2:H:109:PHE:CZ	2.52	0.43
1:I:284:PRO:HB2	1:I:557:PRO:CG	2.48	0.43
1:O:238:LYS:HA	1:O:330:LEU:O	2.19	0.43
1:C:377:LEU:HB3	1:C:378:PRO:HD2	2.00	0.43
1:C:384:THR:OG1	1:C:493:ASP:OD1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:LEU:HD23	1:E:58:ILE:HG21	2.00	0.43
1:E:160:SER:C	1:E:161:ILE:HD12	2.43	0.43
1:E:394:LEU:CD2	1:E:563:MET:CE	2.96	0.43
1:M:622:MET:HA	1:M:622:MET:CE	2.43	0.43
1:O:609:SER:OG	1:O:705:PHE:O	2.36	0.43
1:E:2:LYS:HE2	1:E:2:LYS:HB2	1.85	0.43
1:K:62:LEU:HD23	1:K:348:PHE:CD1	2.53	0.43
1:K:733:LEU:HD23	1:K:742:VAL:HG12	2.00	0.43
1:O:622:MET:HB3	1:O:623:PRO:HD2	2.00	0.43
1:A:393:THR:HA	1:A:396:TYR:CD2	2.54	0.43
1:C:100:LEU:HG	1:C:161:ILE:HD13	2.00	0.43
1:C:733:LEU:HD23	1:C:742:VAL:HG12	2.00	0.43
1:G:475:LEU:C	1:G:475:LEU:HD23	2.43	0.43
1:I:598:ARG:HD3	1:K:182:ARG:O	2.18	0.43
1:I:622:MET:HB3	1:I:623:PRO:HD2	2.00	0.43
1:M:187:PHE:CD1	1:M:191:VAL:HG11	2.53	0.43
1:M:412:GLN:HG2	2:N:71:ARG:HG2	1.99	0.43
1:O:147:VAL:CG2	1:O:199:VAL:HG23	2.49	0.43
2:P:47:GLU:OE1	2:P:60:SER:HB3	2.19	0.43
1:A:577:PRO:HA	1:A:578:PRO:HD3	1.87	0.43
1:C:160:SER:C	1:C:161:ILE:HD12	2.43	0.43
2:D:35:ILE:HD11	2:D:127:VAL:CG1	2.46	0.43
2:H:47:GLU:OE1	2:H:60:SER:HB3	2.19	0.43
1:I:597:ALA:HB2	1:K:578:PRO:HG2	2.01	0.43
1:K:564:GLU:OE1	1:K:585:THR:HG23	2.18	0.43
1:M:126:LEU:HD12	1:M:126:LEU:HA	1.89	0.43
1:M:410:ILE:CD1	1:O:693:PHE:HB3	2.48	0.43
1:M:532:GLU:HB2	1:M:603:ILE:CD1	2.48	0.43
1:M:643:ILE:HD13	1:M:745:MET:CE	2.49	0.43
1:A:611:PHE:O	1:A:684:TYR:HA	2.19	0.43
1:A:622:MET:HB3	1:A:623:PRO:HD2	2.00	0.43
1:C:402:GLU:HG2	1:C:404:ILE:H	1.84	0.43
1:E:516:THR:HG21	1:E:520:PRO:HG3	1.99	0.43
1:G:473:TRP:HA	1:G:473:TRP:CE3	2.54	0.43
1:K:346:PHE:N	1:K:346:PHE:HD1	2.16	0.43
1:M:654:GLY:HA2	1:M:726:SER:OG	2.18	0.43
1:O:393:THR:HA	1:O:396:TYR:CD2	2.53	0.43
1:A:238:LYS:HA	1:A:330:LEU:O	2.18	0.43
1:C:74:GLN:HB2	1:C:230:TRP:CZ3	2.54	0.43
1:I:238:LYS:HA	1:I:330:LEU:O	2.18	0.43
1:I:362:LYS:HG3	1:I:371:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:53:PHE:CE1	2:J:116:MET:HE1	2.54	0.43
1:K:255:GLU:OE1	1:K:259:ARG:NH1	2.45	0.43
1:O:618:TYR:CE2	1:O:642:ARG:HD3	2.54	0.43
1:A:89:GLN:HG3	1:A:89:GLN:O	2.18	0.43
1:C:643:ILE:HD13	1:C:745:MET:CE	2.48	0.43
1:E:40:ARG:NH2	1:E:42:ILE:HD11	2.33	0.43
1:E:377:LEU:HB3	1:E:378:PRO:HD2	2.00	0.43
1:I:125:ASN:HB2	1:I:219:LEU:CD2	2.49	0.43
2:L:104:LEU:HD12	2:L:104:LEU:HA	1.83	0.43
1:O:657:GLU:HB2	1:O:727:ILE:CD1	2.49	0.43
1:O:713:PHE:CE2	1:O:721:MET:HB3	2.54	0.43
2:D:78:ARG:HD3	2:D:123:ARG:NH2	2.34	0.42
1:E:365:TYR:O	1:E:366:GLU:HB2	2.19	0.42
1:E:713:PHE:CZ	1:E:721:MET:HB3	2.54	0.42
1:K:263:VAL:O	1:K:264:ARG:C	2.61	0.42
1:K:306:ARG:HG2	1:K:330:LEU:CD2	2.49	0.42
2:P:73:GLN:O	2:P:78:ARG:NH1	2.50	0.42
1:E:505:ALA:O	1:E:509:ARG:HG3	2.19	0.42
1:E:678:VAL:O	1:E:679:GLU:HB2	2.18	0.42
1:E:703:HIS:CD2	2:H:72:MET:HE1	2.54	0.42
2:F:72:MET:HE3	2:F:72:MET:HB2	1.89	0.42
1:G:371:TYR:CD2	1:G:463:PRO:HD2	2.54	0.42
1:I:192:PRO:HB3	1:K:716:ALA:HB2	2.01	0.42
2:J:124:ILE:O	2:J:127:VAL:HG13	2.19	0.42
1:O:484:TRP:CG	1:O:733:LEU:HD13	2.54	0.42
1:O:570:GLY:HA3	1:O:574:TRP:CZ2	2.54	0.42
1:C:90:PRO:HG2	1:C:94:PHE:CB	2.48	0.42
1:E:643:ILE:HD13	1:E:745:MET:CE	2.49	0.42
1:G:57:ALA:C	1:G:58:ILE:HD12	2.44	0.42
1:K:74:GLN:HB2	1:K:230:TRP:CZ3	2.55	0.42
1:M:2:LYS:HE2	1:M:2:LYS:HB2	1.86	0.42
1:M:23:PHE:HB2	1:M:346:PHE:CD1	2.54	0.42
1:M:318:GLU:OE2	1:O:596:ARG:NE	2.51	0.42
1:M:598:ARG:NH2	1:O:182:ARG:HD3	2.34	0.42
1:O:394:LEU:HD23	1:O:498:HIS:CE1	2.54	0.42
2:P:35:ILE:HD11	2:P:128:ARG:HG2	2.01	0.42
1:A:472:ILE:CD1	1:A:477:ALA:HA	2.50	0.42
1:A:608:MET:HA	1:A:659:ASP:OD1	2.19	0.42
1:A:659:ASP:HB2	1:A:725:SER:HB3	2.01	0.42
1:E:283:ILE:O	1:E:283:ILE:CG2	2.67	0.42
1:E:508:LEU:HD22	1:E:514:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:609:SER:HB3	1:G:658:LEU:O	2.19	0.42
2:H:35:ILE:HD11	2:H:128:ARG:HG2	2.01	0.42
1:C:187:PHE:CD1	1:C:191:VAL:HG11	2.54	0.42
1:E:384:THR:OG1	1:E:493:ASP:OD1	2.36	0.42
1:E:402:GLU:HG2	1:E:404:ILE:HG13	2.00	0.42
1:G:93:ALA:HB2	1:G:167:PRO:CD	2.48	0.42
1:I:43:HIS:CE1	1:I:51:PRO:HG2	2.54	0.42
1:I:700:GLY:HA2	1:I:706:VAL:HG11	2.01	0.42
1:K:629:ARG:HE	1:K:762:VAL:HG13	1.85	0.42
1:M:40:ARG:NH2	1:M:42:ILE:HD11	2.34	0.42
1:A:93:ALA:HB2	1:A:167:PRO:CD	2.49	0.42
1:A:455:ARG:HH22	1:E:294:TYR:HH	1.63	0.42
2:B:49:ALA:HB2	2:B:117:HIS:CE1	2.54	0.42
1:C:179:VAL:O	1:C:179:VAL:HG23	2.19	0.42
1:E:151:ARG:CG	1:E:195:SER:HA	2.50	0.42
2:F:61:PRO:HB2	2:H:61:PRO:HB3	2.01	0.42
1:G:284:PRO:HB2	1:G:557:PRO:CG	2.48	0.42
1:I:393:THR:HA	1:I:396:TYR:CD2	2.55	0.42
1:I:609:SER:HB3	1:I:658:LEU:O	2.19	0.42
1:K:100:LEU:HG	1:K:161:ILE:HD13	2.00	0.42
1:A:75:PHE:O	1:A:234:HIS:NE2	2.53	0.42
1:A:618:TYR:CE2	1:A:642:ARG:HD3	2.55	0.42
1:G:125:ASN:HB2	1:G:219:LEU:CD2	2.50	0.42
1:A:43:HIS:CE1	1:A:51:PRO:HG2	2.55	0.42
1:A:284:PRO:HB2	1:A:557:PRO:CG	2.50	0.42
1:A:394:LEU:CD2	1:A:563:MET:CE	2.94	0.42
1:C:236:ASN:HB3	1:C:445:ASP:OD1	2.18	0.42
1:C:604:TRP:CD1	1:C:721:MET:HE2	2.54	0.42
1:E:733:LEU:HD23	1:E:742:VAL:HG12	2.01	0.42
2:F:73:GLN:HB3	2:F:74:PRO:HD2	2.02	0.42
1:G:238:LYS:HA	1:G:330:LEU:O	2.20	0.42
1:G:393:THR:HA	1:G:396:TYR:CD2	2.55	0.42
2:J:17:ASP:HA	1:K:663:LEU:HD11	2.02	0.42
1:M:38:LEU:HD23	1:M:58:ILE:HG21	2.01	0.42
1:M:100:LEU:HD12	1:M:100:LEU:C	2.44	0.42
1:M:402:GLU:CG	1:M:404:ILE:HG13	2.49	0.42
1:E:572:THR:HB	1:E:574:TRP:HD1	1.84	0.42
1:K:90:PRO:HG2	1:K:94:PHE:CB	2.49	0.42
1:K:572:THR:HB	1:K:574:TRP:HD1	1.85	0.42
1:A:473:TRP:HA	1:A:473:TRP:CE3	2.55	0.42
2:B:120:PHE:CE2	2:B:124:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:THR:OG1	1:E:456:ARG:NH2	2.49	0.42
1:G:331:TRP:CH2	1:G:447:ARG:HG3	2.55	0.42
1:I:577:PRO:HA	1:I:578:PRO:HD3	1.89	0.42
1:K:604:TRP:CD1	1:K:721:MET:HE2	2.54	0.42
1:K:607:GLY:O	1:K:608:MET:C	2.63	0.42
1:M:263:VAL:O	1:M:264:ARG:C	2.63	0.42
1:M:458:ILE:O	1:M:462:ARG:NH1	2.53	0.42
2:P:107:GLU:HG3	2:P:109:PHE:CZ	2.54	0.42
1:C:513:VAL:HA	1:C:540:ARG:O	2.20	0.41
1:I:611:PHE:O	1:I:684:TYR:HA	2.20	0.41
1:I:618:TYR:CE2	1:I:642:ARG:HD3	2.55	0.41
1:K:505:ALA:O	1:K:509:ARG:HG3	2.20	0.41
1:K:513:VAL:HA	1:K:540:ARG:O	2.20	0.41
1:M:691:LYS:NZ	1:O:575:GLU:HG2	2.35	0.41
1:O:125:ASN:HB2	1:O:219:LEU:CD2	2.50	0.41
1:A:394:LEU:CB	1:A:563:MET:HE1	2.50	0.41
1:G:75:PHE:O	1:G:234:HIS:NE2	2.53	0.41
1:G:713:PHE:CE2	1:G:721:MET:HB3	2.55	0.41
1:I:394:LEU:CD2	1:I:563:MET:CE	2.96	0.41
1:K:452:THR:OG1	1:K:456:ARG:NH2	2.53	0.41
1:O:310:GLY:HA3	5:O:903:HOH:O	2.19	0.41
1:O:475:LEU:C	1:O:475:LEU:HD23	2.44	0.41
1:A:394:LEU:HD23	1:A:498:HIS:CE1	2.55	0.41
1:E:179:VAL:O	1:E:179:VAL:HG23	2.20	0.41
1:G:60:SER:O	1:G:63:GLU:HG2	2.20	0.41
1:G:622:MET:HB3	1:G:623:PRO:HD2	2.02	0.41
1:M:597:ALA:HB2	1:O:578:PRO:HG2	2.01	0.41
1:O:57:ALA:C	1:O:58:ILE:HD12	2.45	0.41
2:P:124:ILE:O	2:P:127:VAL:HG13	2.20	0.41
1:C:508:LEU:HD22	1:C:514:VAL:HG21	2.01	0.41
1:G:632:TRP:NE1	1:G:760:PRO:HG2	2.35	0.41
1:K:236:ASN:HB3	1:K:445:ASP:OD1	2.20	0.41
1:K:490:PHE:CE2	1:K:750:LEU:HD23	2.54	0.41
1:M:90:PRO:HG2	1:M:94:PHE:CB	2.51	0.41
1:O:4:ILE:HB	1:O:427:GLU:CG	2.43	0.41
2:B:49:ALA:HB2	2:B:117:HIS:NE2	2.35	0.41
1:G:394:LEU:CD2	1:G:563:MET:CE	2.96	0.41
1:G:399:TYR:CZ	1:G:440:TYR:CZ	3.09	0.41
1:I:394:LEU:CB	1:I:563:MET:HE1	2.50	0.41
1:K:394:LEU:CD2	1:K:563:MET:CE	2.97	0.41
1:M:151:ARG:CG	1:M:195:SER:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:473:TRP:HA	1:O:473:TRP:CE3	2.56	0.41
1:A:519:HIS:HE1	1:A:547:ASN:ND2	2.15	0.41
1:G:183:THR:CG2	1:G:314:ASP:HA	2.51	0.41
1:M:607:GLY:O	1:M:659:ASP:HA	2.21	0.41
1:M:644:GLY:HA3	1:M:653:ALA:HB3	2.02	0.41
1:O:601:GLN:HG3	1:O:606:THR:CA	2.51	0.41
1:A:475:LEU:HD23	1:A:475:LEU:C	2.45	0.41
1:C:26:SER:HB3	1:C:342:TRP:CH2	2.56	0.41
1:E:629:ARG:HE	1:E:762:VAL:HG13	1.86	0.41
1:K:187:PHE:CE1	1:K:191:VAL:HG21	2.56	0.41
1:M:1:MET:CE	2:N:91:ARG:HH12	2.33	0.41
1:A:216:ILE:O	1:A:217:ALA:CB	2.69	0.41
1:E:490:PHE:CE2	1:E:750:LEU:HD23	2.55	0.41
1:I:216:ILE:O	1:I:217:ALA:CB	2.68	0.41
1:I:553:VAL:HG13	1:I:563:MET:CG	2.47	0.41
2:J:107:GLU:HG3	2:J:109:PHE:CZ	2.56	0.41
2:L:78:ARG:HD3	2:L:123:ARG:NH2	2.35	0.41
1:M:733:LEU:HD23	1:M:742:VAL:HG12	2.03	0.41
1:O:179:VAL:HG23	1:O:179:VAL:O	2.21	0.41
1:O:216:ILE:O	1:O:217:ALA:CB	2.69	0.41
1:O:614:ASP:OD2	1:O:681:SER:OG	2.34	0.41
1:O:700:GLY:HA2	1:O:706:VAL:HG11	2.03	0.41
2:D:35:ILE:HD13	2:D:35:ILE:HA	1.91	0.41
1:E:607:GLY:O	1:E:659:ASP:HA	2.21	0.41
1:G:609:SER:OG	1:G:705:PHE:O	2.37	0.41
2:H:43:GLU:H	2:H:43:GLU:CD	2.29	0.41
1:I:519:HIS:CE1	1:I:547:ASN:HB3	2.56	0.41
1:I:570:GLY:HA3	1:I:574:TRP:CZ2	2.56	0.41
1:I:713:PHE:CE2	1:I:721:MET:HB3	2.56	0.41
1:K:103:THR:OG1	1:K:445:ASP:OD1	2.39	0.41
1:K:394:LEU:HD23	1:K:498:HIS:CE1	2.56	0.41
1:K:644:GLY:HA3	1:K:653:ALA:CB	2.50	0.41
1:M:255:GLU:OE1	1:M:259:ARG:NH1	2.43	0.41
1:M:564:GLU:OE1	1:M:585:THR:HG23	2.20	0.41
1:O:611:PHE:O	1:O:684:TYR:HA	2.20	0.41
1:A:394:LEU:C	1:A:563:MET:HE1	2.46	0.41
1:C:685:THR:CG2	1:C:686:VAL:N	2.84	0.41
1:E:187:PHE:CD1	1:E:191:VAL:HG11	2.56	0.41
1:I:608:MET:HA	1:I:659:ASP:OD1	2.21	0.41
1:M:31:ARG:NH1	1:M:366:GLU:OE2	2.54	0.41
1:C:1:MET:CE	2:D:91:ARG:HH12	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:VAL:O	1:E:264:ARG:C	2.64	0.40
1:I:166:ASP:OD2	1:I:169:LYS:HE3	2.21	0.40
1:K:151:ARG:CG	1:K:195:SER:HA	2.50	0.40
1:M:572:THR:HB	1:M:574:TRP:HD1	1.85	0.40
2:N:61:PRO:HB2	2:P:61:PRO:HB3	2.03	0.40
1:A:57:ALA:C	1:A:58:ILE:HD12	2.46	0.40
1:A:125:ASN:HB2	1:A:219:LEU:HD21	2.03	0.40
1:A:371:TYR:CD2	1:A:463:PRO:HD2	2.56	0.40
1:C:263:VAL:O	1:C:264:ARG:C	2.63	0.40
1:E:318:GLU:OE2	1:G:596:ARG:NE	2.53	0.40
1:E:685:THR:CG2	1:E:686:VAL:N	2.84	0.40
1:G:77:SER:HB2	1:G:304:PRO:HD3	2.03	0.40
2:H:35:ILE:HD11	2:H:128:ARG:CG	2.52	0.40
1:I:77:SER:HB2	1:I:304:PRO:HD3	2.04	0.40
1:I:632:TRP:NE1	1:I:760:PRO:HG2	2.35	0.40
1:K:31:ARG:NH1	1:K:366:GLU:OE2	2.53	0.40
1:M:179:VAL:O	1:M:179:VAL:HG23	2.22	0.40
1:K:9:TYR:CE2	1:K:340:CYS:HB2	2.57	0.40
1:K:516:THR:CG2	1:K:517:GLY:N	2.84	0.40
1:K:610:SER:HB2	1:K:685:THR:O	2.22	0.40
1:K:643:ILE:HD13	1:K:745:MET:CE	2.51	0.40
1:M:402:GLU:HG2	1:M:403:GLN:N	2.36	0.40
1:O:394:LEU:O	1:O:563:MET:HE1	2.21	0.40
1:A:632:TRP:NE1	1:A:760:PRO:HG2	2.36	0.40
1:C:31:ARG:NH1	1:C:366:GLU:OE2	2.54	0.40
1:C:607:GLY:O	1:C:659:ASP:HA	2.21	0.40
1:E:634:MET:O	1:E:635:GLU:C	2.65	0.40
1:G:4:ILE:HB	1:G:427:GLU:CG	2.44	0.40
1:G:482:ILE:HD13	1:G:482:ILE:HA	1.91	0.40
1:K:98:LEU:C	1:K:98:LEU:HD12	2.47	0.40
1:M:394:LEU:CD2	1:M:563:MET:CE	2.97	0.40
1:M:582:HIS:ND1	1:M:589:ARG:HA	2.36	0.40
1:C:151:ARG:CG	1:C:195:SER:HA	2.51	0.40
1:C:216:ILE:O	1:C:217:ALA:CB	2.67	0.40
1:C:402:GLU:HG2	1:C:404:ILE:HG13	2.02	0.40
1:E:31:ARG:NH1	1:E:366:GLU:OE2	2.55	0.40
1:E:598:ARG:NH2	1:G:182:ARG:HD3	2.35	0.40
2:F:104:LEU:HA	2:F:104:LEU:HD12	1.80	0.40
1:G:29:GLU:HG3	1:G:31:ARG:HH11	1.86	0.40
1:I:657:GLU:HB2	1:I:727:ILE:CD1	2.52	0.40
1:K:475:LEU:C	1:K:475:LEU:HD23	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:516:THR:HG21	1:M:520:PRO:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	760/775 (98%)	715 (94%)	43 (6%)	2 (0%)	36	66
1	C	760/775 (98%)	715 (94%)	44 (6%)	1 (0%)	48	77
1	E	760/775 (98%)	717 (94%)	42 (6%)	1 (0%)	48	77
1	G	760/775 (98%)	716 (94%)	41 (5%)	3 (0%)	30	60
1	I	760/775 (98%)	716 (94%)	41 (5%)	3 (0%)	30	60
1	K	760/775 (98%)	713 (94%)	46 (6%)	1 (0%)	48	77
1	M	760/775 (98%)	718 (94%)	41 (5%)	1 (0%)	48	77
1	O	760/775 (98%)	718 (94%)	39 (5%)	3 (0%)	30	60
2	B	123/132 (93%)	114 (93%)	8 (6%)	1 (1%)	16	44
2	D	123/132 (93%)	118 (96%)	5 (4%)	0	100	100
2	F	123/132 (93%)	117 (95%)	6 (5%)	0	100	100
2	H	123/132 (93%)	114 (93%)	8 (6%)	1 (1%)	16	44
2	J	123/132 (93%)	114 (93%)	8 (6%)	1 (1%)	16	44
2	L	123/132 (93%)	118 (96%)	5 (4%)	0	100	100
2	N	123/132 (93%)	118 (96%)	5 (4%)	0	100	100
2	P	123/132 (93%)	113 (92%)	10 (8%)	0	100	100
All	All	7064/7256 (97%)	6654 (94%)	392 (6%)	18 (0%)	36	66

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	635	GLU
1	G	635	GLU
1	I	635	GLU
1	O	635	GLU
1	A	761	ARG
1	C	366	GLU
1	E	366	GLU
1	G	761	ARG
1	I	217	ALA
1	I	761	ARG
1	O	761	ARG
2	B	17	ASP
1	G	217	ALA
2	J	17	ASP
1	K	366	GLU
1	M	366	GLU
1	O	217	ALA
2	H	17	ASP

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	621/631 (98%)	595 (96%)	26 (4%)	26	61
1	C	621/631 (98%)	594 (96%)	27 (4%)	26	60
1	E	621/631 (98%)	593 (96%)	28 (4%)	24	58
1	G	621/631 (98%)	593 (96%)	28 (4%)	24	58
1	I	621/631 (98%)	596 (96%)	25 (4%)	28	63
1	K	621/631 (98%)	593 (96%)	28 (4%)	24	58
1	M	621/631 (98%)	593 (96%)	28 (4%)	24	58
1	O	621/631 (98%)	595 (96%)	26 (4%)	26	61
2	B	111/117 (95%)	105 (95%)	6 (5%)	20	51
2	D	111/117 (95%)	103 (93%)	8 (7%)	13	39
2	F	111/117 (95%)	103 (93%)	8 (7%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	111/117 (95%)	105 (95%)	6 (5%)	20	51
2	J	111/117 (95%)	103 (93%)	8 (7%)	13	39
2	L	111/117 (95%)	103 (93%)	8 (7%)	13	39
2	N	111/117 (95%)	103 (93%)	8 (7%)	13	39
2	P	111/117 (95%)	104 (94%)	7 (6%)	16	45
All	All	5856/5984 (98%)	5581 (95%)	275 (5%)	23	57

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	69	ARG
1	A	96	VAL
1	A	150	ASP
1	A	161	ILE
1	A	180	VAL
1	A	186	ARG
1	A	190	VAL
1	A	191	VAL
1	A	195	SER
1	A	264	ARG
1	A	357	ASP
1	A	402	GLU
1	A	410	ILE
1	A	516	THR
1	A	553	VAL
1	A	598	ARG
1	A	620	VAL
1	A	626	GLN
1	A	628	GLU
1	A	657	GLU
1	A	682	VAL
1	A	689	ASP
1	A	691	LYS
1	A	698	MET
1	A	762	VAL
2	B	29	ARG
2	B	35	ILE
2	B	36	ASP
2	B	60	SER

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Mol	Chain	Res	Type
2	B	110	LYS
2	B	127	VAL
1	C	1	MET
1	C	15	VAL
1	C	69	ARG
1	C	91	ASP
1	C	150	ASP
1	C	177	LYS
1	C	180	VAL
1	C	191	VAL
1	C	195	SER
1	C	204	THR
1	C	205	VAL
1	C	226	ASP
1	C	309	THR
1	C	352	GLU
1	C	402	GLU
1	C	516	THR
1	C	553	VAL
1	C	571	VAL
1	C	598	ARG
1	C	603	ILE
1	C	610	SER
1	C	620	VAL
1	C	625	SER
1	C	698	MET
1	C	727	ILE
1	C	744	LYS
1	C	756	ASP
2	D	8	CYS
2	D	29	ARG
2	D	36	ASP
2	D	78	ARG
2	D	104	LEU
2	D	112	GLU
2	D	125	GLU
2	D	127	VAL
1	E	1	MET
1	E	15	VAL
1	E	69	ARG
1	E	91	ASP
1	E	150	ASP

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Mol	Chain	Res	Type
1	E	177	LYS
1	E	180	VAL
1	E	191	VAL
1	E	195	SER
1	E	204	THR
1	E	205	VAL
1	E	226	ASP
1	E	309	THR
1	E	346	PHE
1	E	352	GLU
1	E	402	GLU
1	E	516	THR
1	E	553	VAL
1	E	571	VAL
1	E	598	ARG
1	E	603	ILE
1	E	610	SER
1	E	620	VAL
1	E	625	SER
1	E	698	MET
1	E	727	ILE
1	E	744	LYS
1	E	756	ASP
2	F	8	CYS
2	F	29	ARG
2	F	36	ASP
2	F	78	ARG
2	F	104	LEU
2	F	112	GLU
2	F	125	GLU
2	F	127	VAL
1	G	15	VAL
1	G	69	ARG
1	G	96	VAL
1	G	150	ASP
1	G	161	ILE
1	G	180	VAL
1	G	186	ARG
1	G	190	VAL
1	G	191	VAL
1	G	195	SER
1	G	264	ARG

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Mol	Chain	Res	Type
1	G	402	GLU
1	G	410	ILE
1	G	516	THR
1	G	553	VAL
1	G	598	ARG
1	G	620	VAL
1	G	626	GLN
1	G	628	GLU
1	G	657	GLU
1	G	661	TYR
1	G	682	VAL
1	G	689	ASP
1	G	691	LYS
1	G	698	MET
1	G	750	LEU
1	G	751	ASN
1	G	762	VAL
2	H	29	ARG
2	H	35	ILE
2	H	36	ASP
2	H	60	SER
2	H	110	LYS
2	H	127	VAL
1	I	15	VAL
1	I	69	ARG
1	I	96	VAL
1	I	150	ASP
1	I	161	ILE
1	I	180	VAL
1	I	186	ARG
1	I	190	VAL
1	I	191	VAL
1	I	195	SER
1	I	264	ARG
1	I	402	GLU
1	I	410	ILE
1	I	516	THR
1	I	553	VAL
1	I	598	ARG
1	I	620	VAL
1	I	626	GLN
1	I	628	GLU

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Mol	Chain	Res	Type
1	I	657	GLU
1	I	682	VAL
1	I	689	ASP
1	I	691	LYS
1	I	698	MET
1	I	762	VAL
2	J	29	ARG
2	J	35	ILE
2	J	36	ASP
2	J	60	SER
2	J	72	MET
2	J	74	PRO
2	J	110	LYS
2	J	127	VAL
1	K	1	MET
1	K	15	VAL
1	K	69	ARG
1	K	91	ASP
1	K	150	ASP
1	K	177	LYS
1	K	180	VAL
1	K	191	VAL
1	K	195	SER
1	K	204	THR
1	K	205	VAL
1	K	226	ASP
1	K	309	THR
1	K	346	PHE
1	K	352	GLU
1	K	402	GLU
1	K	516	THR
1	K	553	VAL
1	K	571	VAL
1	K	598	ARG
1	K	603	ILE
1	K	610	SER
1	K	620	VAL
1	K	625	SER
1	K	698	MET
1	K	727	ILE
1	K	744	LYS
1	K	756	ASP

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Mol	Chain	Res	Type
2	L	8	CYS
2	L	29	ARG
2	L	36	ASP
2	L	78	ARG
2	L	104	LEU
2	L	112	GLU
2	L	125	GLU
2	L	127	VAL
1	M	1	MET
1	M	15	VAL
1	M	69	ARG
1	M	91	ASP
1	M	150	ASP
1	M	177	LYS
1	M	180	VAL
1	M	191	VAL
1	M	195	SER
1	M	204	THR
1	M	205	VAL
1	M	226	ASP
1	M	309	THR
1	M	346	PHE
1	M	352	GLU
1	M	402	GLU
1	M	516	THR
1	M	553	VAL
1	M	571	VAL
1	M	598	ARG
1	M	603	ILE
1	M	610	SER
1	M	620	VAL
1	M	625	SER
1	M	698	MET
1	M	727	ILE
1	M	744	LYS
1	M	756	ASP
2	N	8	CYS
2	N	29	ARG
2	N	36	ASP
2	N	78	ARG
2	N	104	LEU
2	N	112	GLU

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Mol	Chain	Res	Type
2	N	125	GLU
2	N	127	VAL
1	O	15	VAL
1	O	69	ARG
1	O	96	VAL
1	O	150	ASP
1	O	161	ILE
1	O	180	VAL
1	O	186	ARG
1	O	190	VAL
1	O	191	VAL
1	O	195	SER
1	O	264	ARG
1	O	402	GLU
1	O	410	ILE
1	O	516	THR
1	O	553	VAL
1	O	598	ARG
1	O	620	VAL
1	O	626	GLN
1	O	628	GLU
1	O	657	GLU
1	O	661	TYR
1	O	682	VAL
1	O	689	ASP
1	O	691	LYS
1	O	698	MET
1	O	762	VAL
2	P	29	ARG
2	P	35	ILE
2	P	36	ASP
2	P	60	SER
2	P	74	PRO
2	P	110	LYS
2	P	127	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	406	HIS
1	A	424	ASN

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Mol	Chain	Res	Type
1	A	465	HIS
1	A	480	HIS
1	A	501	ASN
1	A	519	HIS
2	B	48	HIS
2	B	67	HIS
1	C	121	GLN
1	C	403	GLN
1	C	406	HIS
1	C	480	HIS
1	C	519	HIS
1	C	547	ASN
1	C	626	GLN
2	D	51	ASN
1	E	121	GLN
1	E	406	HIS
1	E	412	GLN
1	E	480	HIS
1	E	519	HIS
1	E	547	ASN
1	E	626	GLN
2	F	51	ASN
1	G	251	GLN
1	G	287	HIS
1	G	406	HIS
1	G	412	GLN
1	G	480	HIS
1	G	501	ASN
1	G	519	HIS
2	H	41	HIS
2	H	48	HIS
2	H	67	HIS
1	I	251	GLN
1	I	333	HIS
1	I	406	HIS
1	I	424	ASN
1	I	465	HIS
1	I	480	HIS
1	I	501	ASN
1	I	519	HIS
1	I	547	ASN
2	J	41	HIS

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Mol	Chain	Res	Type
2	J	48	HIS
2	J	67	HIS
2	J	73	GLN
1	K	121	GLN
1	K	406	HIS
1	K	480	HIS
1	K	519	HIS
1	K	547	ASN
1	K	626	GLN
1	K	741	ASN
2	L	51	ASN
1	M	121	GLN
1	M	406	HIS
1	M	480	HIS
1	M	519	HIS
1	M	547	ASN
1	M	626	GLN
2	N	51	ASN
1	O	251	GLN
1	O	406	HIS
1	O	480	HIS
1	O	501	ASN
1	O	519	HIS
2	P	41	HIS
2	P	48	HIS
2	P	67	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
4	EDO	L	201	-	3,3,3	0.49	0	2,2,2	0.20	0
4	EDO	H	201	-	3,3,3	0.50	0	2,2,2	0.31	0
4	EDO	B	201	-	3,3,3	0.54	0	2,2,2	0.23	0
4	EDO	J	201	-	3,3,3	0.53	0	2,2,2	0.24	0
4	EDO	N	201	-	3,3,3	0.55	0	2,2,2	0.20	0
4	EDO	F	201	-	3,3,3	0.55	0	2,2,2	0.18	0
4	EDO	D	201	-	3,3,3	0.53	0	2,2,2	0.17	0
4	EDO	P	201	-	3,3,3	0.47	0	2,2,2	0.24	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
4	EDO	L	201	-	-	0/1/1/1	-
4	EDO	H	201	-	-	0/1/1/1	-
4	EDO	B	201	-	-	0/1/1/1	-
4	EDO	J	201	-	-	0/1/1/1	-
4	EDO	N	201	-	-	0/1/1/1	-
4	EDO	F	201	-	-	0/1/1/1	-
4	EDO	D	201	-	-	0/1/1/1	-
4	EDO	P	201	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	762/775 (98%)	0.45	29 (3%)	44	35	13, 25, 49, 76	0
1	C	762/775 (98%)	0.55	34 (4%)	38	30	15, 28, 51, 87	0
1	E	762/775 (98%)	0.45	37 (4%)	35	27	13, 26, 49, 81	0
1	G	762/775 (98%)	0.61	45 (5%)	28	21	13, 30, 56, 76	0
1	I	762/775 (98%)	0.52	31 (4%)	41	33	14, 25, 48, 75	0
1	K	762/775 (98%)	0.44	23 (3%)	52	42	13, 26, 49, 81	0
1	M	762/775 (98%)	0.45	31 (4%)	41	33	13, 26, 49, 85	0
1	O	762/775 (98%)	0.51	44 (5%)	29	22	14, 25, 49, 76	0
2	B	125/132 (94%)	0.80	10 (8%)	18	13	24, 33, 53, 62	0
2	D	125/132 (94%)	0.95	8 (6%)	25	18	27, 39, 54, 74	0
2	F	125/132 (94%)	0.96	11 (8%)	15	11	27, 38, 54, 72	0
2	H	125/132 (94%)	0.94	13 (10%)	11	8	28, 36, 57, 65	0
2	J	125/132 (94%)	0.89	10 (8%)	18	13	24, 33, 52, 63	0
2	L	125/132 (94%)	0.92	9 (7%)	21	16	25, 36, 56, 63	0
2	N	125/132 (94%)	0.79	10 (8%)	18	13	23, 36, 54, 70	0
2	P	125/132 (94%)	0.70	3 (2%)	59	49	20, 34, 53, 62	0
All	All	7096/7256 (97%)	0.55	348 (4%)	35	27	13, 28, 52, 87	0

All (348) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	690	ASP	5.1
1	O	690	ASP	5.0
1	G	690	ASP	4.9
1	O	575	GLU	4.9
1	C	367	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	O	1	MET	4.7
1	I	690	ASP	4.6
1	C	690	ASP	4.6
1	C	691	LYS	4.5
1	G	1	MET	4.5
1	M	689	ASP	4.4
1	A	690	ASP	4.3
1	E	1	MET	4.3
1	E	573	ALA	4.3
1	G	575	GLU	4.3
1	E	691	LYS	4.2
1	E	446	GLY	4.2
1	K	367	ASP	4.2
1	C	204	THR	4.2
1	I	1	MET	4.1
1	A	575	GLU	4.1
1	K	1	MET	4.0
1	M	691	LYS	4.0
1	C	225	GLN	4.0
1	O	168	GLU	4.0
2	B	7	SER	4.0
1	I	575	GLU	4.0
1	E	367	ASP	4.0
1	K	689	ASP	4.0
1	G	294	TYR	4.0
1	E	575	GLU	3.9
2	H	7	SER	3.9
1	C	226	ASP	3.9
1	E	150	ASP	3.9
1	M	367	ASP	3.9
1	E	638	ASP	3.9
2	L	7	SER	3.9
1	K	690	ASP	3.8
2	P	28	GLU	3.8
1	O	367	ASP	3.8
1	I	226	ASP	3.7
1	O	573	ALA	3.7
1	G	691	LYS	3.7
1	A	251	GLN	3.6
1	M	575	GLU	3.6
1	O	166	ASP	3.6
1	K	2	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	226	ASP	3.6
1	K	691	LYS	3.6
1	I	594	ARG	3.6
2	F	28	GLU	3.6
2	B	131	LEU	3.6
2	F	62	TYR	3.5
1	O	430	LYS	3.5
1	C	1	MET	3.5
1	C	91	ASP	3.5
2	N	23	TYR	3.5
1	M	225	GLN	3.4
1	I	635	GLU	3.4
1	G	252	ASP	3.4
1	I	91	ASP	3.4
2	P	7	SER	3.4
1	I	371	TYR	3.4
1	E	252	ASP	3.3
1	C	224	ALA	3.3
2	D	37	ILE	3.3
1	M	761	ARG	3.3
1	O	689	ASP	3.2
1	O	688	PRO	3.2
1	K	575	GLU	3.2
1	A	573	ALA	3.2
2	N	125	GLU	3.2
1	M	2	LYS	3.2
1	I	227	GLY	3.2
1	I	691	LYS	3.1
2	J	8	CYS	3.1
1	M	91	ASP	3.1
1	O	226	ASP	3.1
2	J	36	ASP	3.1
2	N	78	ARG	3.1
1	E	2	LYS	3.1
1	A	446	GLY	3.1
1	O	691	LYS	3.1
2	D	7	SER	3.1
2	D	36	ASP	3.1
2	J	28	GLU	3.1
1	O	225	GLN	3.0
1	M	690	ASP	3.0
1	K	594	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	J	29	ARG	3.0
2	F	23	TYR	3.0
1	A	691	LYS	3.0
1	G	594	ARG	3.0
1	O	170	LYS	3.0
1	M	226	ASP	3.0
2	J	7	SER	3.0
1	C	352	GLU	3.0
1	C	576	ALA	3.0
1	K	225	GLN	3.0
1	I	689	ASP	3.0
1	E	761	ARG	2.9
1	A	168	GLU	2.9
1	A	594	ARG	2.9
1	A	61	ASP	2.9
1	M	252	ASP	2.9
1	C	506	GLU	2.9
1	K	506	GLU	2.9
1	M	762	VAL	2.9
1	G	225	GLN	2.8
1	A	294	TYR	2.8
1	G	635	GLU	2.8
1	K	294	TYR	2.8
1	K	635	GLU	2.8
1	M	638	ASP	2.8
2	F	107	GLU	2.8
1	I	252	ASP	2.8
2	B	36	ASP	2.8
1	O	473	TRP	2.8
1	O	576	ALA	2.8
1	K	226	ASP	2.8
1	E	352	GLU	2.8
1	E	506	GLU	2.8
1	M	224	ALA	2.8
1	O	294	TYR	2.8
1	C	689	ASP	2.8
1	C	228	ARG	2.7
1	I	761	ARG	2.7
2	N	7	SER	2.7
1	M	626	GLN	2.7
2	F	78	ARG	2.7
2	B	8	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	87	TRP	2.7
1	E	636	GLY	2.7
2	F	7	SER	2.7
2	H	115	ALA	2.7
1	G	169	LYS	2.7
1	A	761	ARG	2.7
1	C	353	GLY	2.7
1	E	91	ASP	2.7
2	L	11	ASP	2.7
2	N	36	ASP	2.7
2	D	46	GLU	2.7
1	A	224	ALA	2.7
1	O	761	ARG	2.7
1	G	636	GLY	2.7
1	M	572	THR	2.7
1	A	63	GLU	2.7
1	E	568	GLU	2.7
2	F	125	GLU	2.7
1	C	594	ARG	2.6
1	G	91	ASP	2.6
1	G	170	LYS	2.6
1	G	491	GLU	2.6
1	M	352	GLU	2.6
1	O	628	GLU	2.6
2	J	46	GLU	2.6
2	L	85	ARG	2.6
2	H	8	CYS	2.6
1	G	142	GLY	2.6
1	O	293	GLY	2.6
2	L	36	ASP	2.6
1	E	227	GLY	2.6
2	B	46	GLU	2.6
1	E	415	ALA	2.6
1	E	445	ASP	2.6
2	N	62	TYR	2.6
2	D	131	LEU	2.6
1	G	20	THR	2.6
1	C	640	GLU	2.6
1	M	281	ASN	2.6
1	I	85	ASP	2.6
1	O	150	ASP	2.6
2	H	110	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	758	PRO	2.5
1	E	294	TYR	2.5
1	C	571	VAL	2.5
1	C	299	ARG	2.5
1	C	170	LYS	2.5
1	O	227	GLY	2.5
1	O	572	THR	2.5
1	G	689	ASP	2.5
2	H	106	ASP	2.5
1	O	178	SER	2.5
1	C	574	TRP	2.5
1	K	628	GLU	2.5
1	G	573	ALA	2.5
1	I	628	GLU	2.5
1	O	255	GLU	2.5
2	H	46	GLU	2.5
2	N	28	GLU	2.5
1	E	368	THR	2.5
1	A	701	GLY	2.4
1	C	636	GLY	2.4
1	M	625	SER	2.4
1	O	129	GLU	2.4
1	I	573	ALA	2.4
2	L	23	TYR	2.4
2	J	106	ASP	2.4
1	G	686	VAL	2.4
2	N	10	ARG	2.4
2	J	23	TYR	2.4
1	G	227	GLY	2.4
2	F	27	ASP	2.4
1	O	568	GLU	2.4
2	D	28	GLU	2.4
1	G	27	ALA	2.4
1	I	578	PRO	2.4
1	E	594	ARG	2.4
1	G	756	ASP	2.4
1	A	635	GLU	2.4
1	M	635	GLU	2.4
1	G	368	THR	2.4
1	E	206	LYS	2.3
2	F	110	LYS	2.3
1	E	226	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	35	ASP	2.3
1	O	737	ASP	2.3
1	O	207	ALA	2.3
1	G	473	TRP	2.3
1	C	206	LYS	2.3
1	C	760	PRO	2.3
1	M	594	ARG	2.3
1	G	130	ASP	2.3
1	M	506	GLU	2.3
2	F	36	ASP	2.3
2	N	111	THR	2.3
1	K	206	LYS	2.3
1	E	281	ASN	2.3
1	A	628	GLU	2.3
1	C	635	GLU	2.3
1	E	635	GLU	2.3
1	I	366	GLU	2.3
1	I	576	ALA	2.3
1	O	491	GLU	2.3
1	O	635	GLU	2.3
2	B	100	GLU	2.3
1	M	445	ASP	2.3
1	K	572	THR	2.3
1	K	762	VAL	2.3
1	K	446	GLY	2.3
1	C	143	ALA	2.3
2	L	28	GLU	2.3
1	O	196	ASP	2.3
1	G	4	ILE	2.3
1	K	761	ARG	2.3
2	B	85	ARG	2.3
2	P	23	TYR	2.3
1	C	227	GLY	2.3
1	A	252	ASP	2.2
1	O	638	ASP	2.2
1	O	687	ILE	2.2
1	C	761	ARG	2.2
2	L	78	ARG	2.2
1	I	572	THR	2.2
2	F	72	MET	2.2
1	O	640	GLU	2.2
1	G	739	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	688	PRO	2.2
2	B	23	TYR	2.2
1	A	246	GLY	2.2
1	E	744	LYS	2.2
1	G	576	ALA	2.2
2	L	125	GLU	2.2
1	G	751	ASN	2.2
2	H	29	ARG	2.2
1	A	91	ASP	2.2
1	A	199	VAL	2.2
1	E	760	PRO	2.2
2	J	9	VAL	2.2
1	I	294	TYR	2.2
1	O	14	SER	2.2
1	G	437	LEU	2.2
1	E	692	ALA	2.2
1	M	223	ALA	2.2
1	O	415	ALA	2.2
1	E	637	ILE	2.2
1	G	588	ARG	2.2
1	A	226	ASP	2.2
1	A	688	PRO	2.2
1	E	3	ASP	2.2
1	I	150	ASP	2.2
1	K	537	ASP	2.2
2	H	102	PRO	2.2
1	G	628	GLU	2.2
1	I	631	ALA	2.2
1	M	168	GLU	2.2
1	O	352	GLU	2.2
2	H	85	ARG	2.1
1	K	756	ASP	2.1
1	C	163	GLY	2.1
1	I	489	GLY	2.1
1	K	647	GLY	2.1
2	B	105	GLY	2.1
1	C	294	TYR	2.1
2	D	69	TYR	2.1
1	O	734	SER	2.1
1	E	628	GLU	2.1
1	I	679	GLU	2.1
1	G	762	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	760	PRO	2.1
1	O	762	VAL	2.1
1	C	3	ASP	2.1
2	H	36	ASP	2.1
1	I	692	ALA	2.1
1	G	63	GLU	2.1
1	K	352	GLU	2.1
2	J	107	GLU	2.1
1	I	762	VAL	2.1
1	A	202	ASP	2.1
1	O	202	ASP	2.1
1	G	759	ALA	2.1
1	A	581	TYR	2.1
1	A	640	GLU	2.1
2	H	86	GLU	2.1
2	N	83	SER	2.1
1	E	225	GLN	2.1
1	A	170	LYS	2.1
1	G	59	LYS	2.1
2	B	110	LYS	2.1
1	E	688	PRO	2.1
1	I	688	PRO	2.1
1	I	537	ASP	2.1
1	M	130	ASP	2.1
1	G	675	ALA	2.1
1	O	692	ALA	2.1
1	G	352	GLU	2.1
1	I	568	GLU	2.1
2	L	40	GLU	2.1
1	G	53	TYR	2.1
1	M	294	TYR	2.1
1	A	1	MET	2.0
1	E	626	GLN	2.0
1	G	167	PRO	2.0
1	O	353	GLY	2.0
1	A	689	ASP	2.0
1	I	687	ILE	2.0
2	H	88	ASP	2.0
1	M	568	GLU	2.0
1	M	581	TYR	2.0
1	C	377	LEU	2.0
1	G	486	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	68	ASN	2.0
1	G	353	GLY	2.0
1	E	572	THR	2.0
1	G	33	THR	2.0
1	M	744	LYS	2.0
1	O	366	GLU	2.0
1	A	574	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

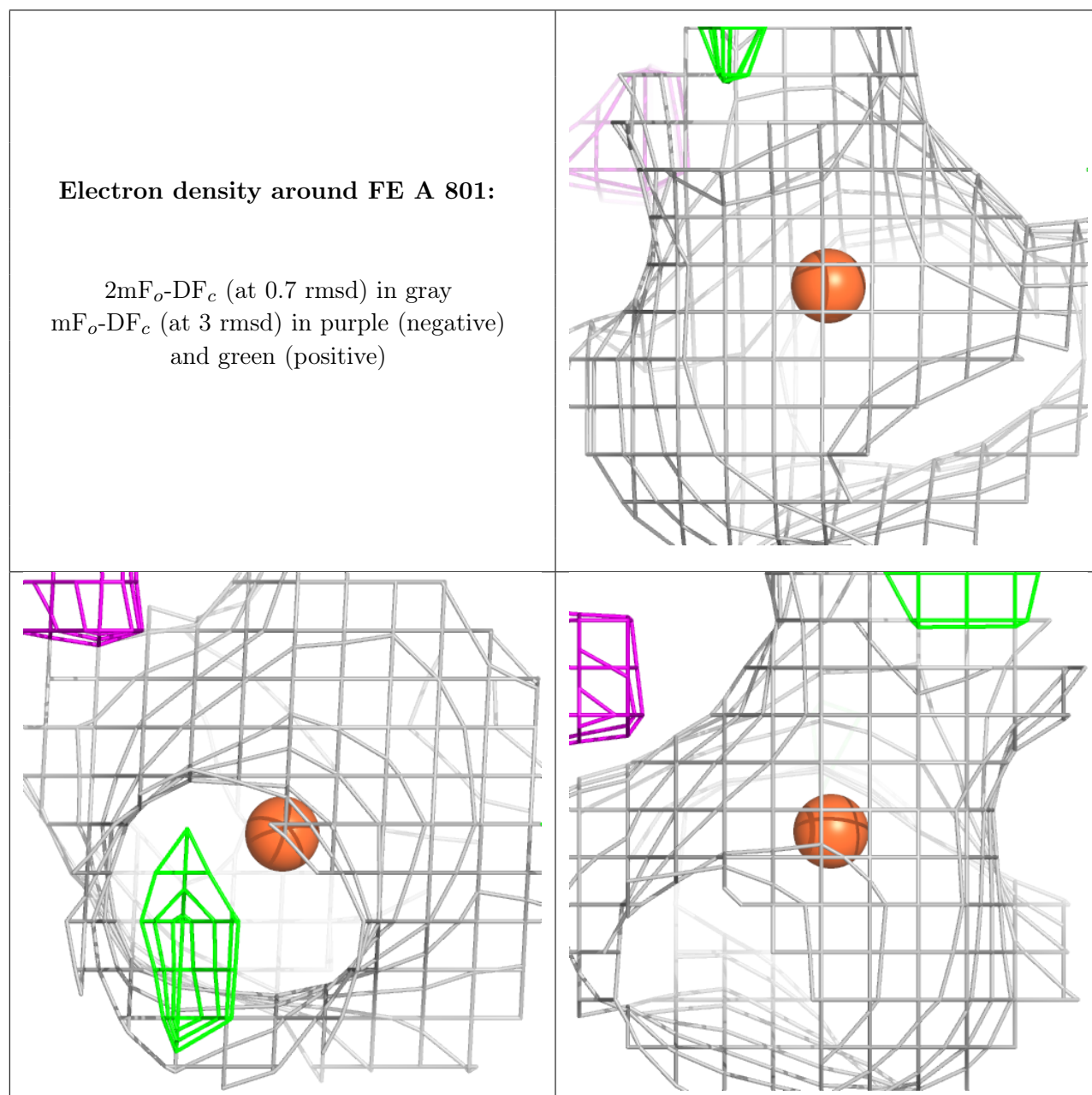
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

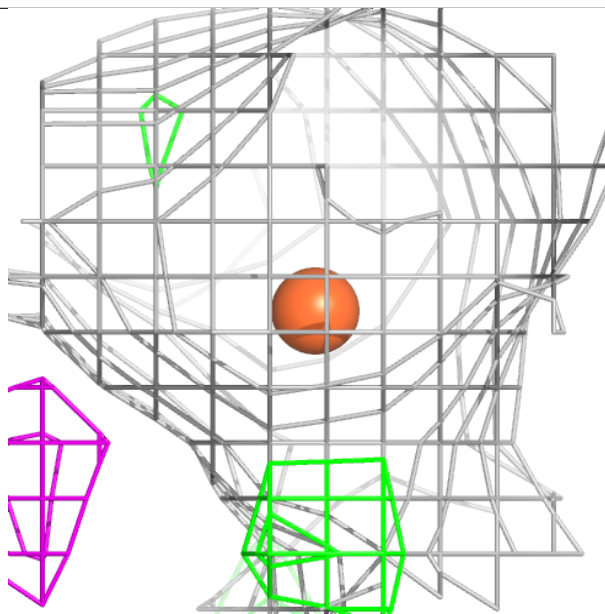
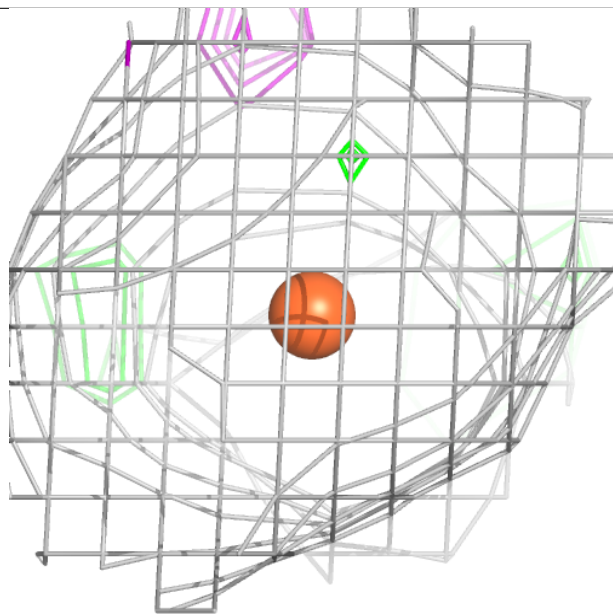
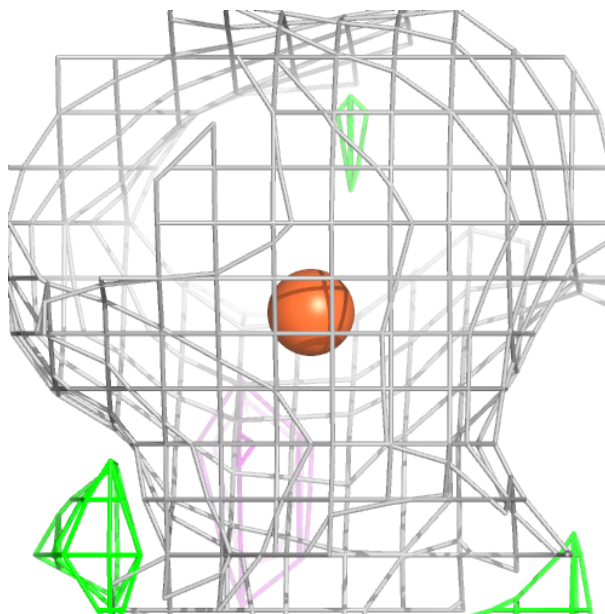
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	F	201	4/4	0.81	0.16	24,31,37,37	0
4	EDO	D	201	4/4	0.85	0.15	18,29,35,35	0
4	EDO	B	201	4/4	0.85	0.13	19,24,32,32	0
4	EDO	H	201	4/4	0.87	0.11	19,23,30,36	0
4	EDO	P	201	4/4	0.87	0.12	15,21,26,26	0
4	EDO	N	201	4/4	0.88	0.11	18,24,30,30	0
4	EDO	J	201	4/4	0.89	0.12	15,24,30,36	0
4	EDO	L	201	4/4	0.91	0.10	16,29,36,36	0
3	FE	A	801	1/1	0.97	0.04	24,24,24,24	0
3	FE	G	801	1/1	0.98	0.03	23,23,23,23	0
3	FE	I	801	1/1	0.99	0.06	21,21,21,21	0
3	FE	K	801	1/1	0.99	0.05	17,17,17,17	0
3	FE	M	801	1/1	0.99	0.02	20,20,20,20	0
3	FE	O	801	1/1	0.99	0.03	23,23,23,23	0
3	FE	E	801	1/1	1.00	0.01	17,17,17,17	0
3	FE	C	801	1/1	1.00	0.02	17,17,17,17	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.



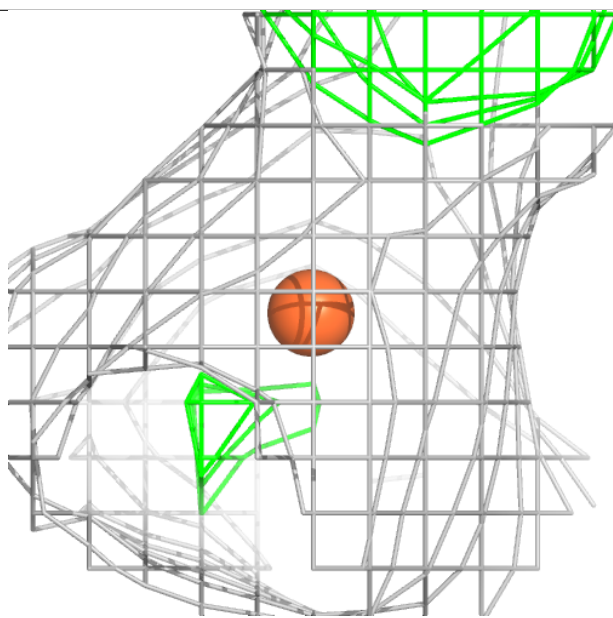
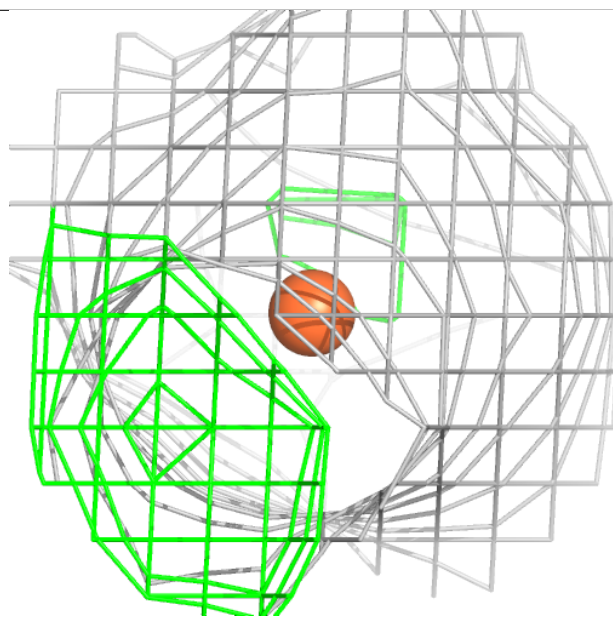
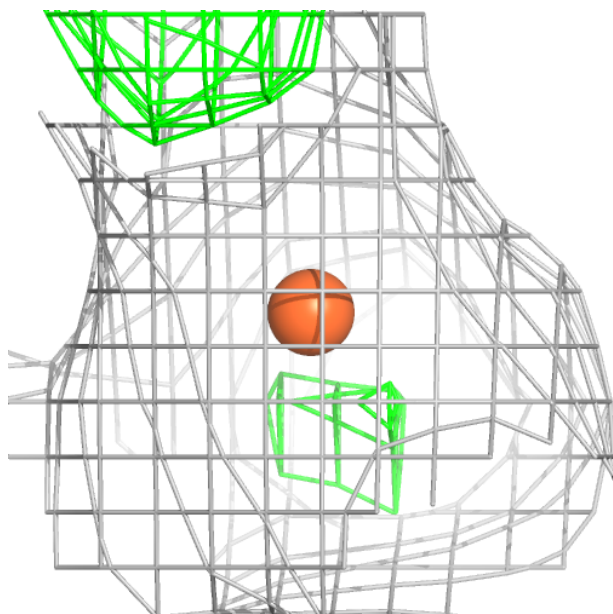
Electron density around FE G 801:

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



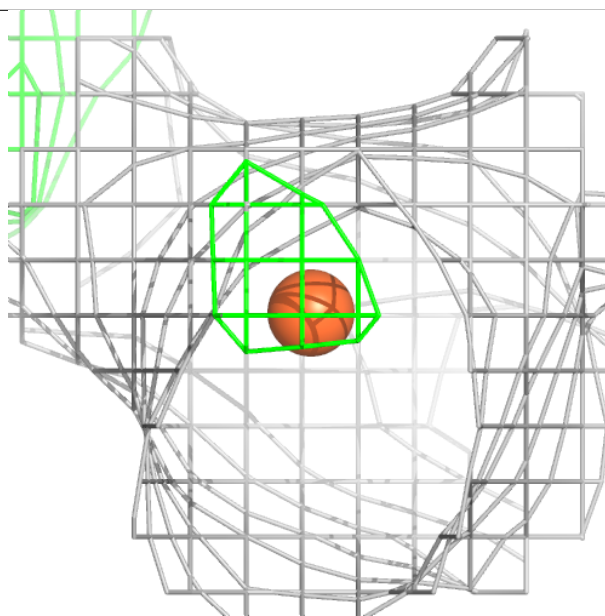
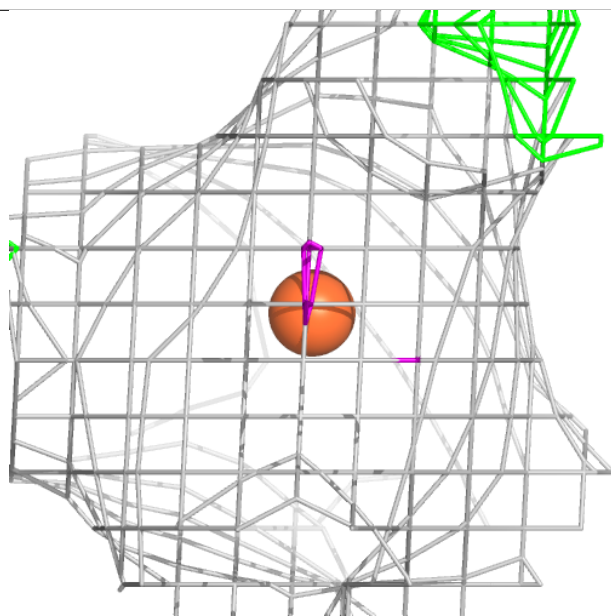
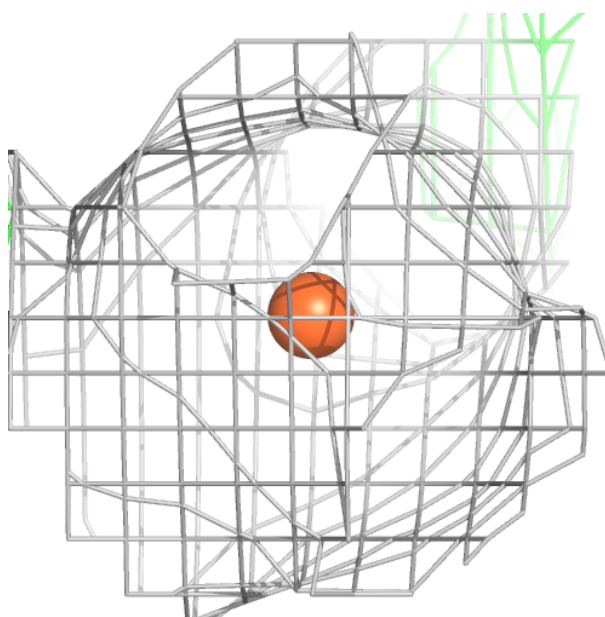
Electron density around FE I 801:

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



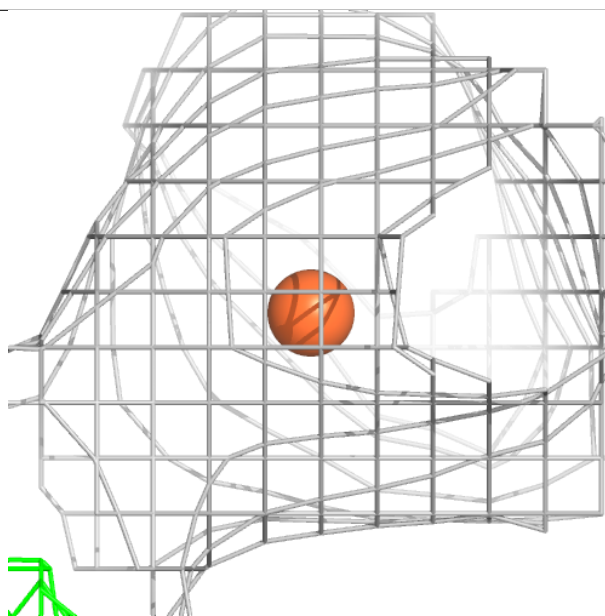
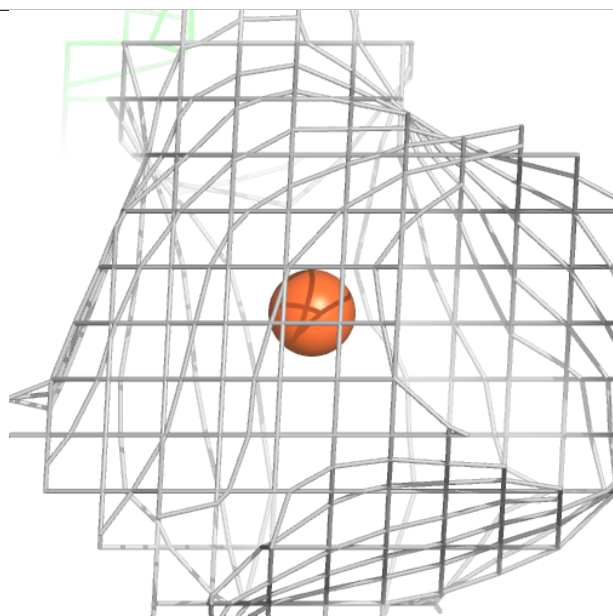
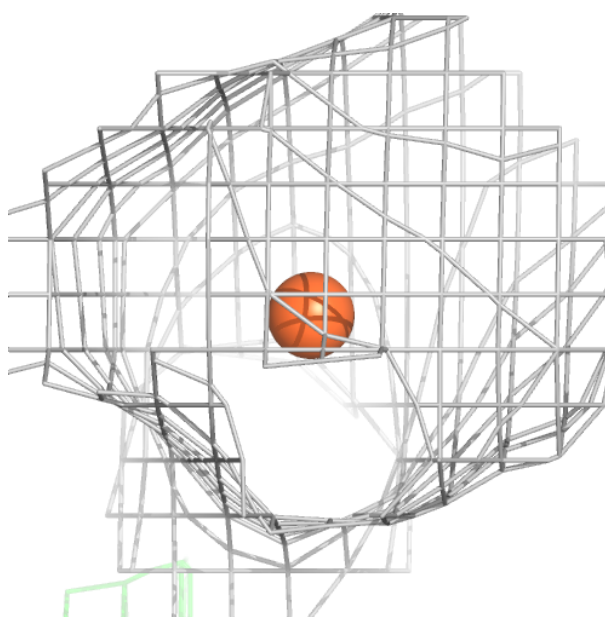
Electron density around FE K 801:

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



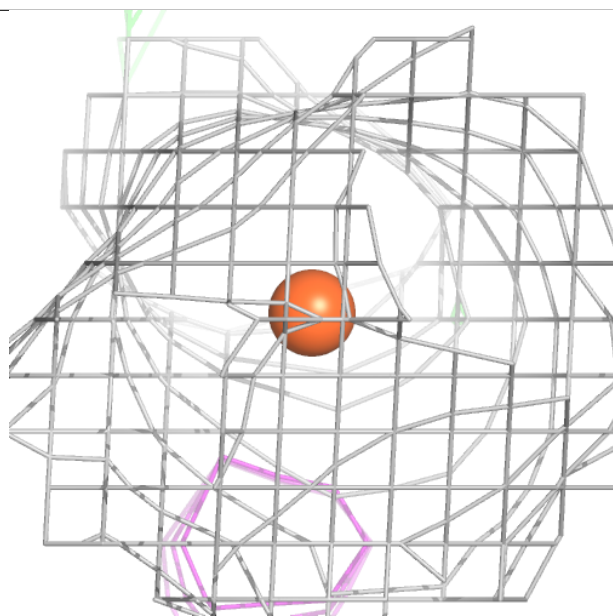
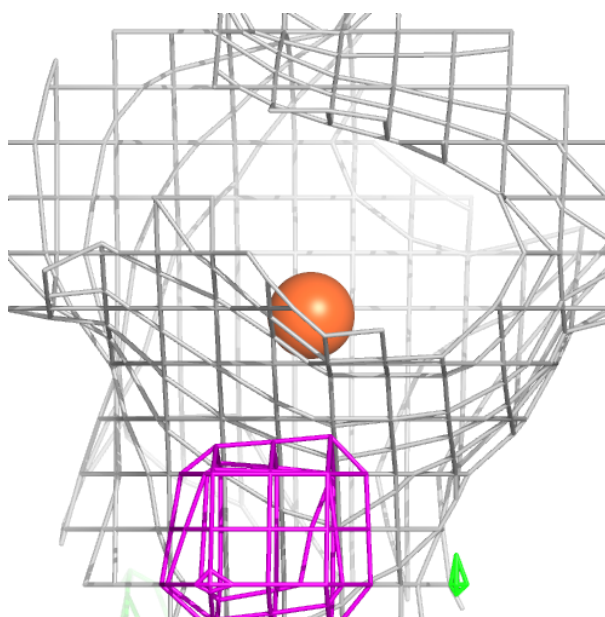
Electron density around FE M 801:

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



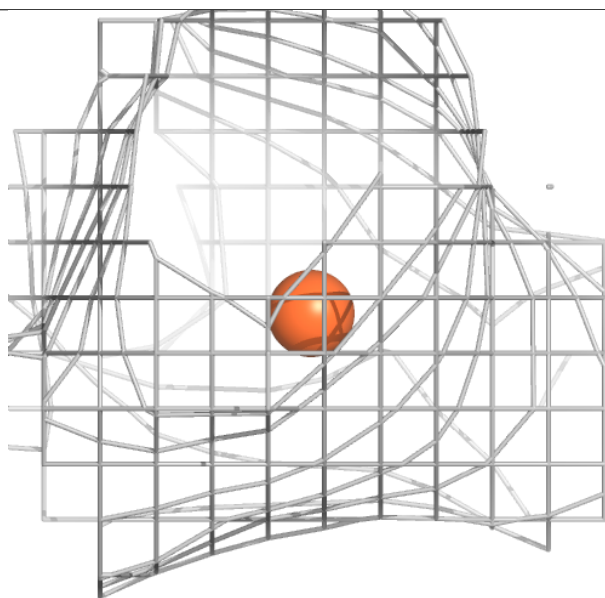
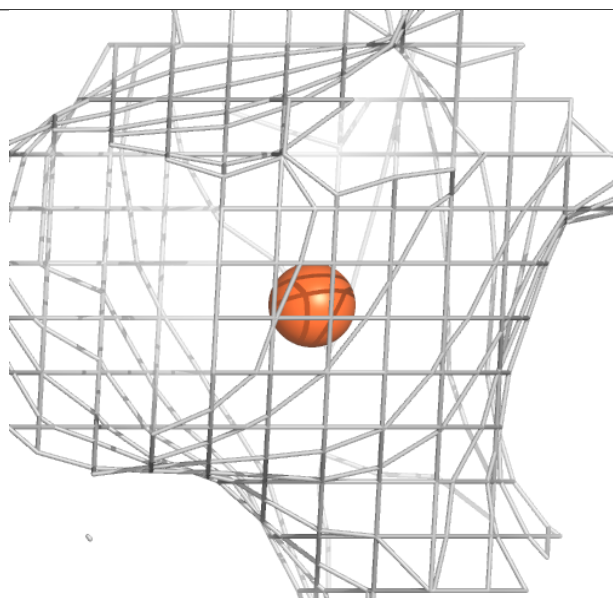
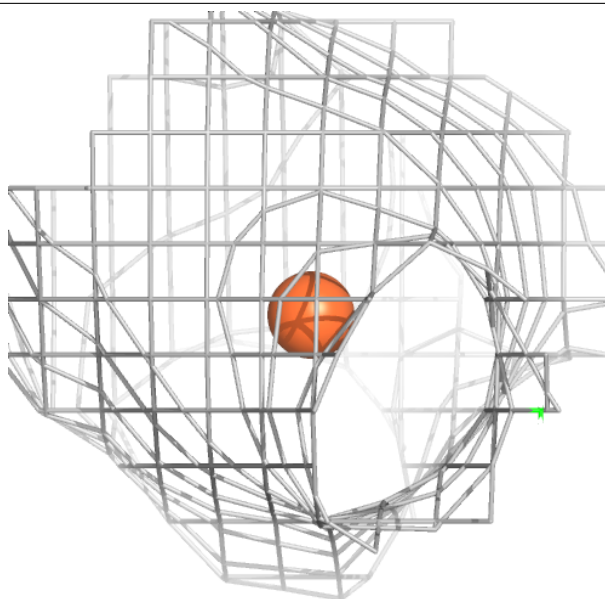
Electron density around FE O 801:

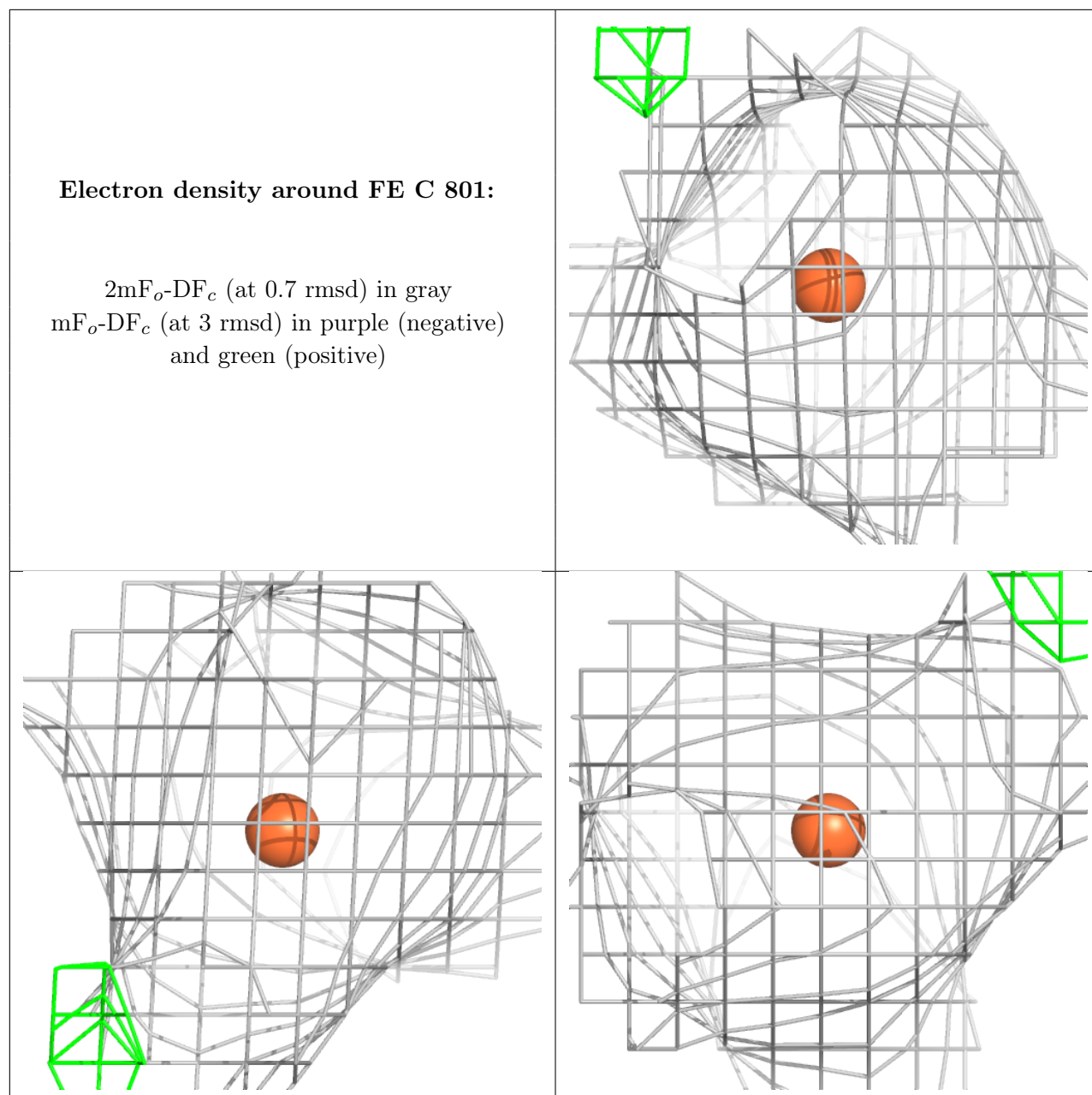
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE E 801:

$2mF_o-DF_c$ (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.