Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 09:33 PM JST

PDB ID	:	6K1G
Title	:	Crystal structure of the L-fucose isomerase soaked with Mn2+ from Raoultella sp.
Authors	:	Kim, I.J.; Kim, D.H.; Nam, K.H.; Kim, K.H.
Deposited on	:	2019-05-10
Resolution	:	2.96 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
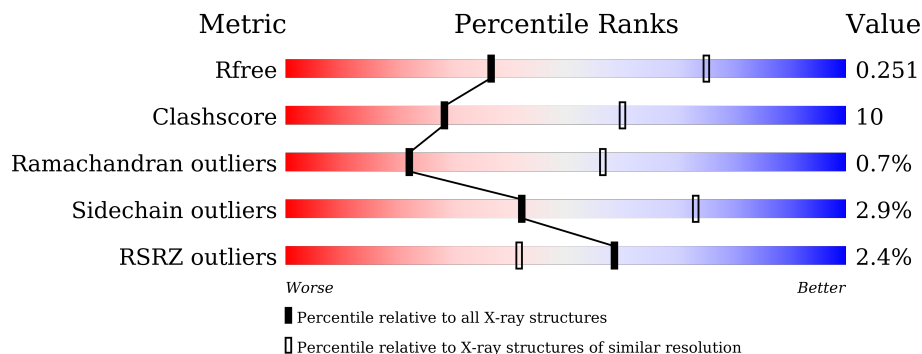
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	612	.% 77% 18% · ·
1	B	612	2% 77% 18% ·
1	C	612	3% 70% 25% · ·
1	D	612	78% 16% · ·
1	E	612	3% 70% 25% · ·
1	F	612	4% 66% 28% · ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 27118 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called L-fucose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	0	0
			4508	2826	790	857	35			
1	B	586	Total	C	N	O	S	0	0	0
			4508	2826	790	857	35			
1	C	586	Total	C	N	O	S	0	0	0
			4508	2826	790	857	35			
1	D	586	Total	C	N	O	S	0	0	0
			4508	2826	790	857	35			
1	E	586	Total	C	N	O	S	0	0	0
			4508	2826	790	857	35			
1	F	586	Total	C	N	O	S	0	0	0
			4508	2826	790	857	35			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A377T0E7
A	-19	GLY	-	expression tag	UNP A0A377T0E7
A	-18	SER	-	expression tag	UNP A0A377T0E7
A	-17	SER	-	expression tag	UNP A0A377T0E7
A	-16	HIS	-	expression tag	UNP A0A377T0E7
A	-15	HIS	-	expression tag	UNP A0A377T0E7
A	-14	HIS	-	expression tag	UNP A0A377T0E7
A	-13	HIS	-	expression tag	UNP A0A377T0E7
A	-12	HIS	-	expression tag	UNP A0A377T0E7
A	-11	HIS	-	expression tag	UNP A0A377T0E7
A	-10	SER	-	expression tag	UNP A0A377T0E7
A	-9	SER	-	expression tag	UNP A0A377T0E7
A	-8	GLY	-	expression tag	UNP A0A377T0E7
A	-7	LEU	-	expression tag	UNP A0A377T0E7
A	-6	VAL	-	expression tag	UNP A0A377T0E7
A	-5	PRO	-	expression tag	UNP A0A377T0E7
A	-4	ARG	-	expression tag	UNP A0A377T0E7

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0A377T0E7
A	-2	SER	-	expression tag	UNP A0A377T0E7
A	-1	HIS	-	expression tag	UNP A0A377T0E7
A	0	MET	-	expression tag	UNP A0A377T0E7
B	-20	MET	-	initiating methionine	UNP A0A377T0E7
B	-19	GLY	-	expression tag	UNP A0A377T0E7
B	-18	SER	-	expression tag	UNP A0A377T0E7
B	-17	SER	-	expression tag	UNP A0A377T0E7
B	-16	HIS	-	expression tag	UNP A0A377T0E7
B	-15	HIS	-	expression tag	UNP A0A377T0E7
B	-14	HIS	-	expression tag	UNP A0A377T0E7
B	-13	HIS	-	expression tag	UNP A0A377T0E7
B	-12	HIS	-	expression tag	UNP A0A377T0E7
B	-11	HIS	-	expression tag	UNP A0A377T0E7
B	-10	SER	-	expression tag	UNP A0A377T0E7
B	-9	SER	-	expression tag	UNP A0A377T0E7
B	-8	GLY	-	expression tag	UNP A0A377T0E7
B	-7	LEU	-	expression tag	UNP A0A377T0E7
B	-6	VAL	-	expression tag	UNP A0A377T0E7
B	-5	PRO	-	expression tag	UNP A0A377T0E7
B	-4	ARG	-	expression tag	UNP A0A377T0E7
B	-3	GLY	-	expression tag	UNP A0A377T0E7
B	-2	SER	-	expression tag	UNP A0A377T0E7
B	-1	HIS	-	expression tag	UNP A0A377T0E7
B	0	MET	-	expression tag	UNP A0A377T0E7
C	-20	MET	-	initiating methionine	UNP A0A377T0E7
C	-19	GLY	-	expression tag	UNP A0A377T0E7
C	-18	SER	-	expression tag	UNP A0A377T0E7
C	-17	SER	-	expression tag	UNP A0A377T0E7
C	-16	HIS	-	expression tag	UNP A0A377T0E7
C	-15	HIS	-	expression tag	UNP A0A377T0E7
C	-14	HIS	-	expression tag	UNP A0A377T0E7
C	-13	HIS	-	expression tag	UNP A0A377T0E7
C	-12	HIS	-	expression tag	UNP A0A377T0E7
C	-11	HIS	-	expression tag	UNP A0A377T0E7
C	-10	SER	-	expression tag	UNP A0A377T0E7
C	-9	SER	-	expression tag	UNP A0A377T0E7
C	-8	GLY	-	expression tag	UNP A0A377T0E7
C	-7	LEU	-	expression tag	UNP A0A377T0E7
C	-6	VAL	-	expression tag	UNP A0A377T0E7
C	-5	PRO	-	expression tag	UNP A0A377T0E7
C	-4	ARG	-	expression tag	UNP A0A377T0E7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP A0A377T0E7
C	-2	SER	-	expression tag	UNP A0A377T0E7
C	-1	HIS	-	expression tag	UNP A0A377T0E7
C	0	MET	-	expression tag	UNP A0A377T0E7
D	-20	MET	-	initiating methionine	UNP A0A377T0E7
D	-19	GLY	-	expression tag	UNP A0A377T0E7
D	-18	SER	-	expression tag	UNP A0A377T0E7
D	-17	SER	-	expression tag	UNP A0A377T0E7
D	-16	HIS	-	expression tag	UNP A0A377T0E7
D	-15	HIS	-	expression tag	UNP A0A377T0E7
D	-14	HIS	-	expression tag	UNP A0A377T0E7
D	-13	HIS	-	expression tag	UNP A0A377T0E7
D	-12	HIS	-	expression tag	UNP A0A377T0E7
D	-11	HIS	-	expression tag	UNP A0A377T0E7
D	-10	SER	-	expression tag	UNP A0A377T0E7
D	-9	SER	-	expression tag	UNP A0A377T0E7
D	-8	GLY	-	expression tag	UNP A0A377T0E7
D	-7	LEU	-	expression tag	UNP A0A377T0E7
D	-6	VAL	-	expression tag	UNP A0A377T0E7
D	-5	PRO	-	expression tag	UNP A0A377T0E7
D	-4	ARG	-	expression tag	UNP A0A377T0E7
D	-3	GLY	-	expression tag	UNP A0A377T0E7
D	-2	SER	-	expression tag	UNP A0A377T0E7
D	-1	HIS	-	expression tag	UNP A0A377T0E7
D	0	MET	-	expression tag	UNP A0A377T0E7
E	-20	MET	-	initiating methionine	UNP A0A377T0E7
E	-19	GLY	-	expression tag	UNP A0A377T0E7
E	-18	SER	-	expression tag	UNP A0A377T0E7
E	-17	SER	-	expression tag	UNP A0A377T0E7
E	-16	HIS	-	expression tag	UNP A0A377T0E7
E	-15	HIS	-	expression tag	UNP A0A377T0E7
E	-14	HIS	-	expression tag	UNP A0A377T0E7
E	-13	HIS	-	expression tag	UNP A0A377T0E7
E	-12	HIS	-	expression tag	UNP A0A377T0E7
E	-11	HIS	-	expression tag	UNP A0A377T0E7
E	-10	SER	-	expression tag	UNP A0A377T0E7
E	-9	SER	-	expression tag	UNP A0A377T0E7
E	-8	GLY	-	expression tag	UNP A0A377T0E7
E	-7	LEU	-	expression tag	UNP A0A377T0E7
E	-6	VAL	-	expression tag	UNP A0A377T0E7
E	-5	PRO	-	expression tag	UNP A0A377T0E7
E	-4	ARG	-	expression tag	UNP A0A377T0E7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP A0A377T0E7
E	-2	SER	-	expression tag	UNP A0A377T0E7
E	-1	HIS	-	expression tag	UNP A0A377T0E7
E	0	MET	-	expression tag	UNP A0A377T0E7
F	-20	MET	-	initiating methionine	UNP A0A377T0E7
F	-19	GLY	-	expression tag	UNP A0A377T0E7
F	-18	SER	-	expression tag	UNP A0A377T0E7
F	-17	SER	-	expression tag	UNP A0A377T0E7
F	-16	HIS	-	expression tag	UNP A0A377T0E7
F	-15	HIS	-	expression tag	UNP A0A377T0E7
F	-14	HIS	-	expression tag	UNP A0A377T0E7
F	-13	HIS	-	expression tag	UNP A0A377T0E7
F	-12	HIS	-	expression tag	UNP A0A377T0E7
F	-11	HIS	-	expression tag	UNP A0A377T0E7
F	-10	SER	-	expression tag	UNP A0A377T0E7
F	-9	SER	-	expression tag	UNP A0A377T0E7
F	-8	GLY	-	expression tag	UNP A0A377T0E7
F	-7	LEU	-	expression tag	UNP A0A377T0E7
F	-6	VAL	-	expression tag	UNP A0A377T0E7
F	-5	PRO	-	expression tag	UNP A0A377T0E7
F	-4	ARG	-	expression tag	UNP A0A377T0E7
F	-3	GLY	-	expression tag	UNP A0A377T0E7
F	-2	SER	-	expression tag	UNP A0A377T0E7
F	-1	HIS	-	expression tag	UNP A0A377T0E7
F	0	MET	-	expression tag	UNP A0A377T0E7

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0
2	E	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0
3	B	9	Total 9	O 9	0	0
3	C	13	Total 13	O 13	0	0
3	D	15	Total 15	O 15	0	0
3	E	5	Total 5	O 5	0	0
3	F	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

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

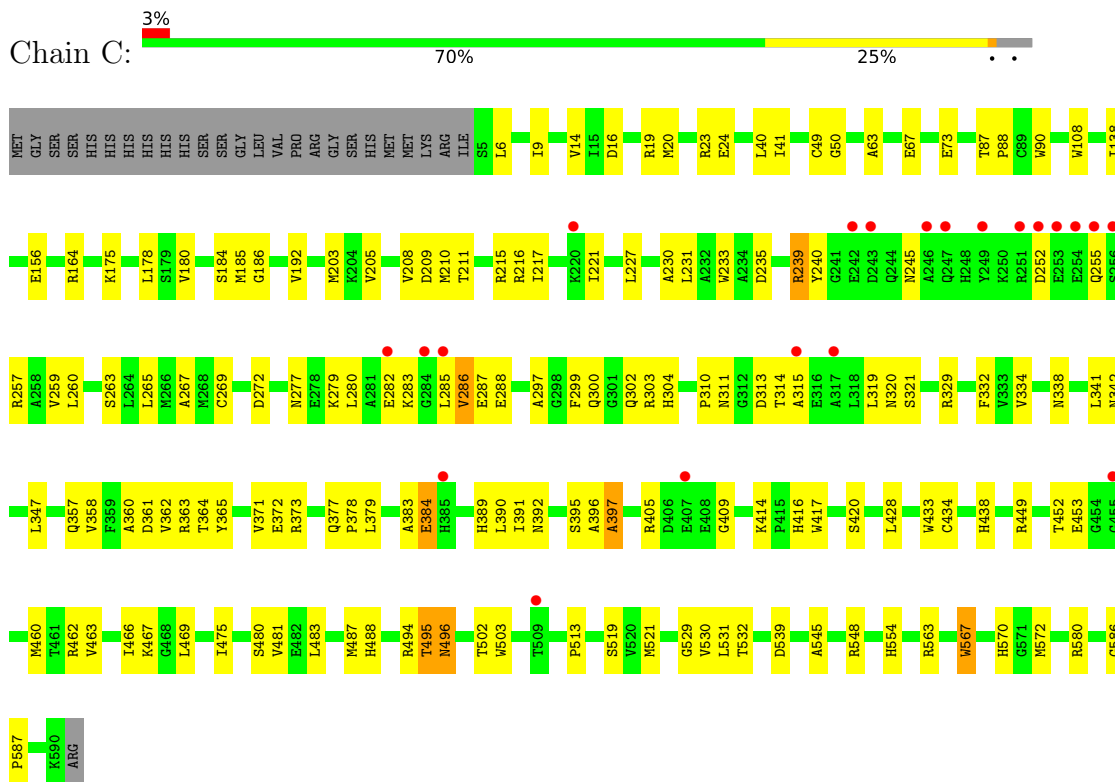- Molecule 1: L-fucose isomerase
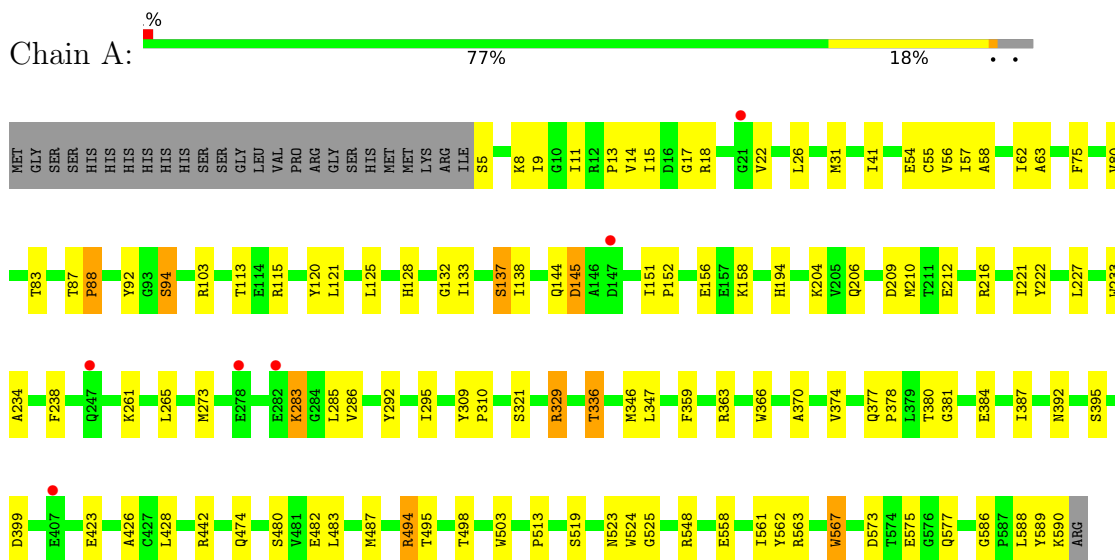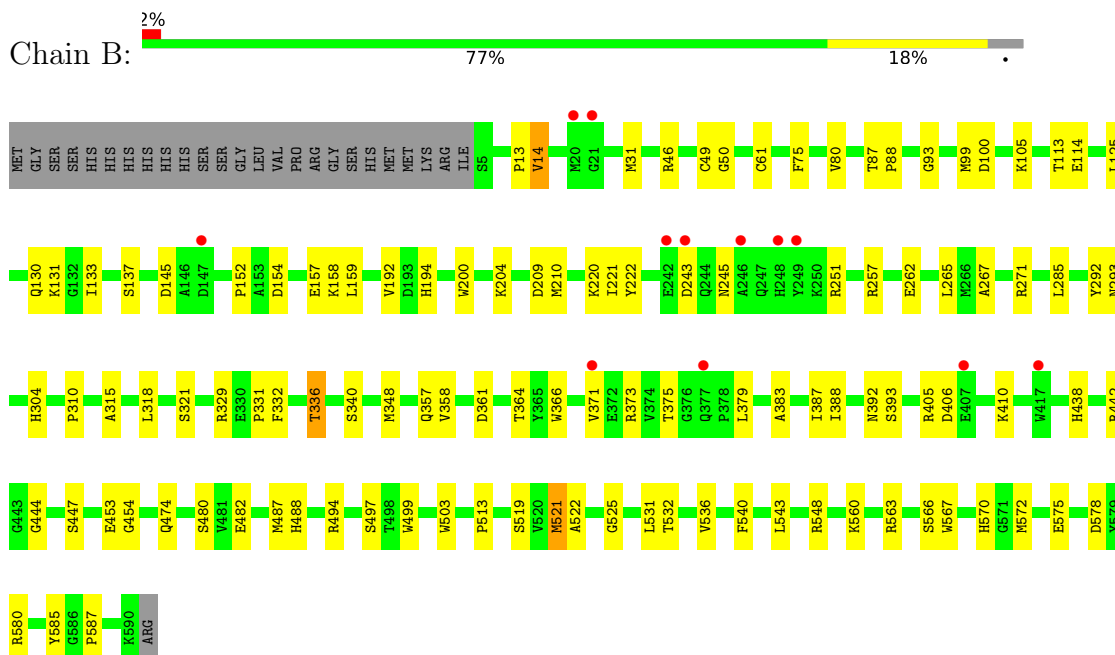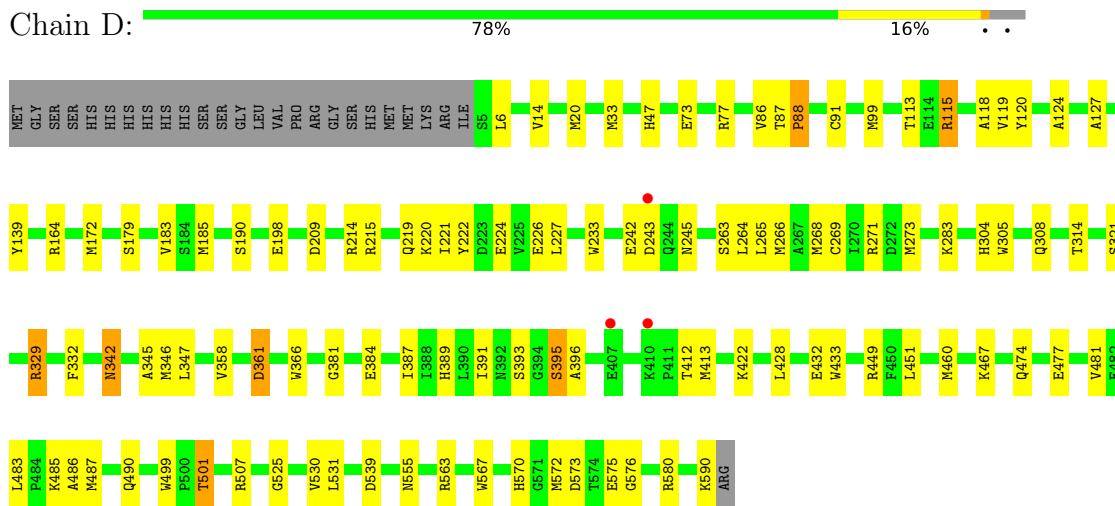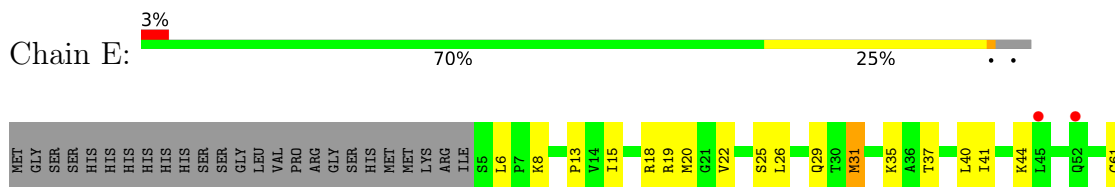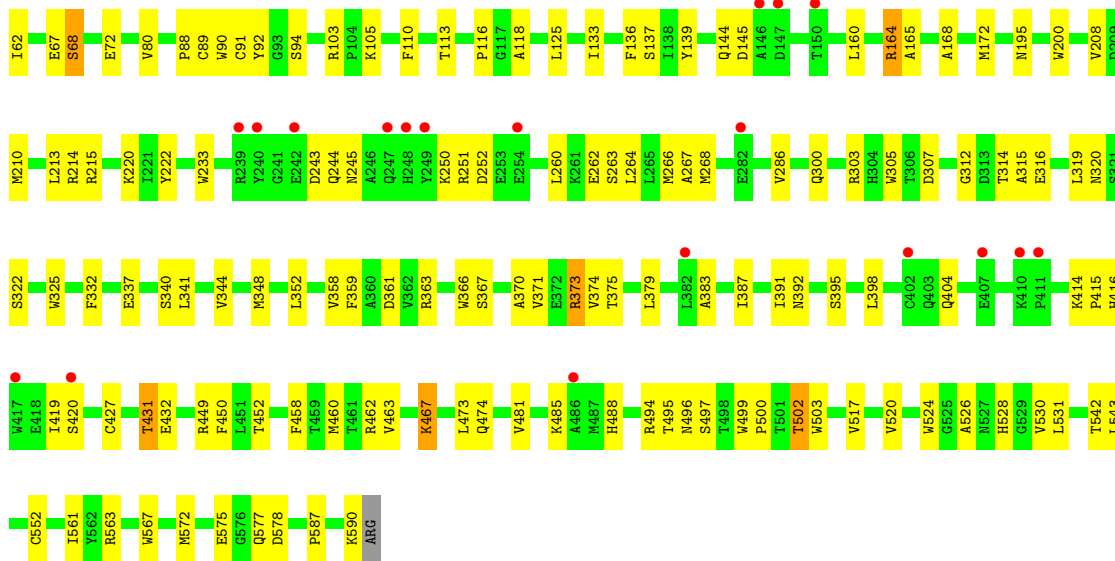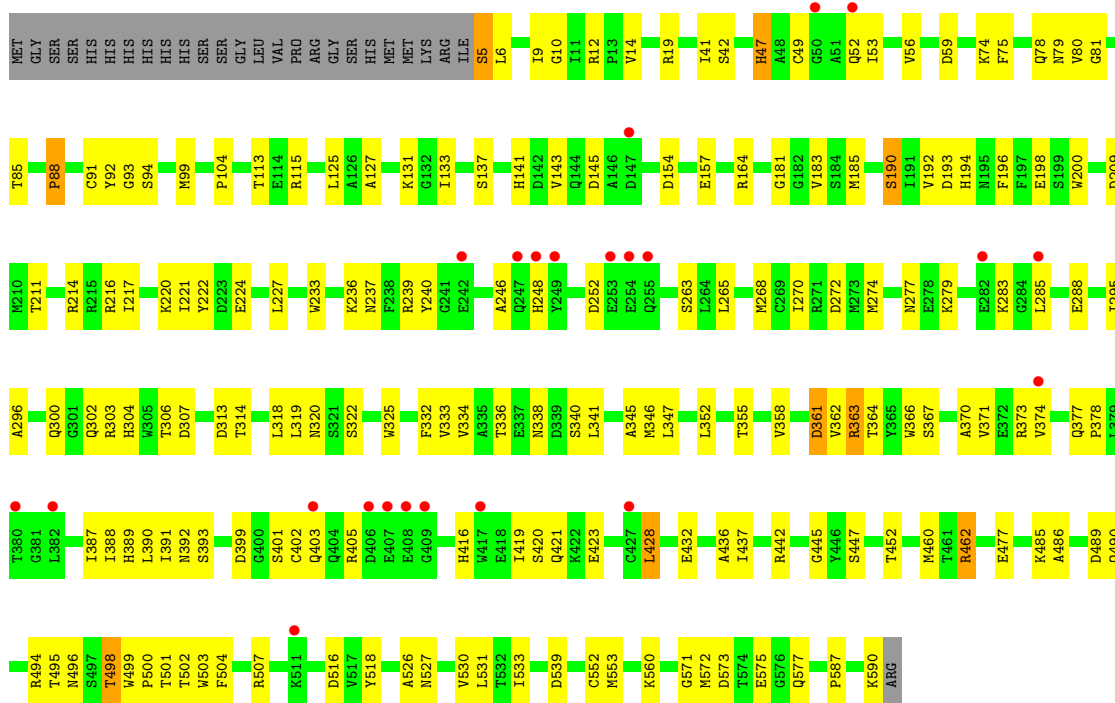

- Molecule 1: L-fucose isomerase

- Molecule 1: L-fucose isomerase

Chain C:

- Molecule 1: L-fucose isomerase

Chain D:

- Molecule 1: L-fucose isomerase

Chain E:

• Molecule 1: L-fucose isomerase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.27Å 163.28Å 196.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.96 29.90 – 2.96	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-2.96) 93.7 (29.90-2.96)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.85 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.189 , 0.252 0.193 , 0.251	Depositor DCC
R_{free} test set	3760 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.9	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27118	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5　Model quality ⓘ

5.1　Standard geometry ⓘ

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

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	0.54	0/4609	0.69	0/6247
1	B	0.51	0/4609	0.67	1/6247 (0.0%)
1	C	0.51	0/4609	0.68	0/6247
1	D	0.52	0/4609	0.67	0/6247
1	E	0.48	0/4609	0.67	0/6247
1	F	0.49	0/4609	0.67	0/6247
All	All	0.51	0/27654	0.68	1/37482 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	361	ASP	CB-CG-OD1	-6.61	112.35	118.30

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	4508	0	4372	75	2
1	B	4508	0	4372	68	0
1	C	4508	0	4372	120	1
1	D	4508	0	4372	73	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4508	0	4372	120	0
1	F	4508	0	4372	130	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	19	0	0	1	0
3	B	9	0	0	0	0
3	C	13	0	0	1	0
3	D	15	0	0	0	0
3	E	5	0	0	1	0
3	F	3	0	0	1	0
All	All	27118	0	26232	521	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (521) 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:C:434:CYS:SG	1:C:449:ARG:NH1	2.17	1.17
1:B:366:TRP:HB2	1:B:387:ILE:HG22	1.42	1.02
1:C:19:ARG:HD2	1:E:286:VAL:HG23	1.52	0.89
1:C:357:GLN:OE1	1:C:532:THR:OG1	1.96	0.83
1:E:366:TRP:HB2	1:E:387:ILE:HG22	1.58	0.82
1:E:61:CYS:O	1:E:67:GLU:OE1	1.98	0.82
1:D:570:HIS:O	1:D:580:ARG:NH1	2.14	0.81
1:E:398:LEU:HD22	1:E:431:THR:HG21	1.62	0.80
1:F:387:ILE:HD11	1:F:503:TRP:HB3	1.64	0.79
1:F:183:VAL:HA	1:F:190:SER:HB2	1.65	0.78
1:C:19:ARG:HD2	1:E:286:VAL:CG2	2.16	0.76
1:C:263:SER:OG	1:C:314:THR:HB	1.85	0.76
1:C:286:VAL:HG23	1:E:19:ARG:NE	1.99	0.76
1:F:355:THR:HG21	1:F:533:ILE:HG21	1.69	0.75
1:B:100:ASP:O	1:B:105:LYS:NZ	2.18	0.75
1:D:77:ARG:HH21	1:D:77:ARG:HB2	1.51	0.75
1:B:570:HIS:O	1:B:580:ARG:NH1	2.19	0.75
1:C:342:ASN:ND2	1:C:529:GLY:O	2.19	0.74
1:B:14:VAL:HG12	1:B:87:THR:HB	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:358:VAL:HB	1:E:531:LEU:HB2	1.69	0.74
1:F:263:SER:HB3	1:F:314:THR:HB	1.69	0.74
1:C:405:ARG:O	1:C:414:LYS:HE2	1.87	0.74
1:C:216:ARG:HA	1:C:221:ILE:HD12	1.68	0.74
1:A:233:TRP:CZ2	1:A:428:LEU:HD11	2.22	0.73
1:D:14:VAL:HG12	1:D:91:CYS:SG	2.29	0.73
1:F:363:ARG:NH2	1:F:496:ASN:OD1	2.22	0.73
1:C:245:ASN:HD21	1:C:438:HIS:H	1.37	0.73
1:E:379:LEU:HD22	1:E:383:ALA:HB1	1.70	0.73
1:E:563:ARG:HD3	1:E:567:TRP:CD1	2.23	0.73
1:B:125:LEU:HD11	1:B:137:SER:HB2	1.70	0.71
1:E:316:GLU:O	1:E:320:ASN:ND2	2.23	0.71
1:F:358:VAL:HG11	1:F:531:LEU:HD12	1.70	0.71
1:A:145:ASP:OD1	1:C:373:ARG:NH2	2.24	0.71
1:E:404:GLN:NE2	1:E:414:LYS:HG2	2.05	0.70
1:D:358:VAL:HB	1:D:531:LEU:HB2	1.74	0.70
1:C:357:GLN:HE22	1:C:532:THR:HG23	1.56	0.70
1:C:211:THR:OG1	1:F:304:HIS:O	2.09	0.69
1:E:145:ASP:OD1	1:F:494:ARG:NH2	2.25	0.69
1:E:160:LEU:O	1:E:164:ARG:HG3	1.92	0.68
1:E:363:ARG:NH1	1:E:496:ASN:OD1	2.25	0.68
1:E:432:GLU:OE1	1:E:449:ARG:NH2	2.23	0.68
1:D:224:GLU:HG3	1:D:283:LYS:NZ	2.09	0.68
1:C:434:CYS:HG	1:C:449:ARG:HH12	1.42	0.67
1:F:217:ILE:HG23	1:F:265:LEU:HD13	1.76	0.67
1:D:366:TRP:HB2	1:D:387:ILE:HG22	1.77	0.67
1:F:239:ARG:HB3	1:F:432:GLU:HG3	1.77	0.67
1:F:391:ILE:HD11	1:F:499:TRP:HB2	1.77	0.67
1:F:185:MET:SD	1:F:302:GLN:HB2	2.36	0.66
1:A:14:VAL:HG12	1:A:62:ILE:HB	1.78	0.66
1:C:548:ARG:HD3	1:C:586:GLY:O	1.96	0.66
1:B:494:ARG:NH2	1:F:145:ASP:OD1	2.29	0.66
1:A:366:TRP:HB2	1:A:387:ILE:HG22	1.78	0.65
1:E:344:VAL:O	1:E:348:MET:HG2	1.96	0.65
1:F:322:SER:OG	1:F:399:ASP:OD2	2.13	0.65
1:A:125:LEU:HD11	1:A:137:SER:HB2	1.78	0.65
1:A:392:ASN:ND2	1:A:395:SER:O	2.24	0.65
1:C:363:ARG:HG3	1:C:364:THR:OG1	1.96	0.65
1:A:227:LEU:HD21	1:A:261:LYS:HE3	1.77	0.65
1:C:240:TYR:OH	1:C:260:LEU:CD1	2.45	0.65
1:C:40:LEU:HD21	1:C:156:GLU:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:GLN:NE2	1:E:497:SER:OG	2.29	0.64
1:E:125:LEU:HD11	1:E:137:SER:HB2	1.80	0.64
1:D:233:TRP:CZ2	1:D:428:LEU:HD11	2.32	0.64
1:D:73:GLU:HG3	1:D:77:ARG:HH11	1.63	0.64
1:B:572:MET:N	1:E:575:GLU:OE1	2.30	0.63
1:C:572:MET:N	1:D:575:GLU:OE2	2.31	0.63
1:E:260:LEU:O	1:E:264:LEU:HD12	1.98	0.63
1:C:342:ASN:OD1	1:C:462:ARG:NH1	2.32	0.63
1:C:49:CYS:O	1:C:416:HIS:NE2	2.28	0.63
1:A:558:GLU:HA	1:A:561:ILE:HG13	1.81	0.63
1:E:213:LEU:HD23	1:E:305:TRP:CH2	2.34	0.63
1:F:221:ILE:HG23	1:F:285:LEU:HD13	1.80	0.62
1:C:481:VAL:HG13	3:C:713:HOH:O	1.98	0.62
1:E:200:TRP:CZ2	1:E:587:PRO:HG3	2.33	0.62
1:F:336:THR:HG21	1:F:392:ASN:HD21	1.64	0.62
1:F:157:GLU:OE2	1:F:560:LYS:NZ	2.32	0.62
1:E:22:VAL:O	1:E:26:LEU:HD12	2.00	0.61
1:A:295:ILE:HD12	1:A:347:LEU:HD11	1.82	0.61
1:C:495:THR:C	1:C:496:ASN:HD22	2.04	0.61
1:E:404:GLN:HE21	1:E:414:LYS:HG2	1.65	0.61
1:A:381:GLY:O	1:A:384:GLU:HB2	2.00	0.61
1:C:209:ASP:OD2	1:F:181:GLY:HA2	2.01	0.61
1:F:125:LEU:HD11	1:F:137:SER:HB2	1.82	0.61
1:E:359:PHE:O	1:E:392:ASN:ND2	2.34	0.61
1:C:14:VAL:HG12	1:C:87:THR:HB	1.83	0.60
1:A:575:GLU:OE1	1:D:572:MET:N	2.34	0.60
1:B:371:VAL:HG11	1:B:379:LEU:HG	1.82	0.60
1:D:183:VAL:HG13	1:D:190:SER:HB2	1.83	0.60
1:F:362:VAL:HG12	1:F:527:ASN:O	2.02	0.60
1:A:144:GLN:OE1	1:A:152:PRO:HG3	2.02	0.60
1:A:8:LYS:HG2	1:A:54:GLU:HB2	1.82	0.59
1:D:224:GLU:HG3	1:D:283:LYS:HZ1	1.67	0.59
1:C:496:ASN:HD22	1:C:496:ASN:N	2.01	0.59
1:D:381:GLY:O	1:D:384:GLU:HB2	2.03	0.59
1:F:263:SER:HB3	1:F:314:THR:CB	2.33	0.59
1:B:262:GLU:OE2	1:B:310:PRO:HD2	2.02	0.59
1:D:226:GLU:HB3	1:D:268:MET:HE1	1.83	0.59
1:F:272:ASP:OD1	1:F:277:ASN:HB2	2.02	0.59
1:B:480:SER:HA	1:B:503:TRP:O	2.02	0.59
1:F:390:LEU:HD11	1:F:504:PHE:HB2	1.84	0.59
1:C:377:GLN:OE1	1:C:487:MET:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:PRO:O	1:D:115:ARG:HB3	2.03	0.59
1:E:145:ASP:OD1	1:F:373:ARG:NH2	2.36	0.59
1:C:341:LEU:HB2	1:C:462:ARG:NH2	2.17	0.58
1:F:272:ASP:CG	1:F:277:ASN:HB2	2.24	0.58
1:E:374:VAL:HG13	1:E:375:THR:HG23	1.86	0.57
1:F:590:LYS:C	3:F:701:HOH:O	2.42	0.57
1:D:73:GLU:HG3	1:D:77:ARG:NH1	2.19	0.57
1:F:377:GLN:HE22	1:F:486:ALA:HB3	1.70	0.57
1:F:233:TRP:CZ2	1:F:428:LEU:HD11	2.39	0.57
1:B:375:THR:HG21	1:B:487:MET:HG3	1.85	0.57
1:B:566:SER:OG	1:B:585:TYR:OH	2.21	0.57
1:E:300:GLN:O	1:E:337:GLU:HA	2.04	0.57
1:F:318:LEU:HD13	1:F:325:TRP:HZ3	1.70	0.57
1:C:286:VAL:HG23	1:E:19:ARG:CD	2.35	0.57
1:C:341:LEU:HB3	1:C:463:VAL:O	2.05	0.57
1:D:33:MET:CE	1:D:86:VAL:HB	2.35	0.57
1:A:221:ILE:HG23	1:A:285:LEU:HD13	1.87	0.56
1:A:17:GLY:HA2	1:A:63:ALA:HB1	1.87	0.56
1:C:460:MET:HA	1:C:530:VAL:O	2.05	0.56
1:D:467:LYS:HE2	1:E:195:ASN:OD1	2.06	0.56
1:B:222:TYR:CE1	1:B:265:LEU:HD21	2.40	0.56
1:F:192:VAL:HG22	1:F:340:SER:OG	2.05	0.56
1:A:87:THR:HG21	1:A:120:TYR:CD2	2.41	0.56
1:C:453:GLU:O	1:C:480:SER:OG	2.19	0.56
1:E:260:LEU:HD13	1:E:264:LEU:CD1	2.35	0.56
1:A:8:LYS:HG2	1:A:54:GLU:O	2.05	0.56
1:C:372:GLU:HG2	1:C:378:PRO:HA	1.87	0.56
1:E:379:LEU:HB3	1:E:383:ALA:O	2.05	0.56
1:C:360:ALA:HB1	1:C:390:LEU:HB3	1.88	0.56
1:E:416:HIS:HA	1:E:419:ILE:HD12	1.88	0.56
1:A:336:THR:HG21	1:A:392:ASN:HD21	1.69	0.55
1:B:192:VAL:HG22	1:B:340:SER:HB3	1.88	0.55
1:B:222:TYR:CD1	1:B:265:LEU:HD21	2.42	0.55
1:C:63:ALA:N	1:C:67:GLU:OE1	2.39	0.55
1:C:227:LEU:HG	1:C:231:LEU:HD11	1.88	0.55
1:E:387:ILE:HD11	1:E:481:VAL:HG21	1.88	0.55
1:A:113:THR:OG1	1:C:494:ARG:HB3	2.06	0.55
1:E:8:LYS:O	1:E:80:VAL:HA	2.06	0.55
1:C:297:ALA:O	1:C:334:VAL:HA	2.05	0.55
1:A:494:ARG:NH1	1:D:113:THR:OG1	2.39	0.55
1:C:184:SER:HB2	1:C:300:GLN:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:GLU:OE2	1:D:507:ARG:NH2	2.32	0.55
1:F:14:VAL:HG12	1:F:91:CYS:SG	2.47	0.55
1:B:373:ARG:NH2	1:F:143:VAL:O	2.38	0.54
1:C:240:TYR:OH	1:C:260:LEU:HD12	2.07	0.54
1:C:545:ALA:HB2	1:C:563:ARG:HG2	1.89	0.54
1:E:341:LEU:HD22	1:E:463:VAL:HG12	1.88	0.54
1:E:572:MET:SD	1:F:553:MET:HA	2.47	0.54
1:B:114:GLU:OE2	1:E:494:ARG:NH1	2.40	0.54
1:C:314:THR:HG23	1:C:433:TRP:CZ3	2.42	0.54
1:A:92:TYR:OH	1:C:303:ARG:NH1	2.41	0.54
1:D:563:ARG:HD3	1:D:567:TRP:CD1	2.43	0.54
1:C:260:LEU:HD23	1:C:260:LEU:O	2.08	0.54
1:F:460:MET:HA	1:F:530:VAL:O	2.08	0.54
1:A:204:LYS:HE2	1:F:99:MET:HG3	1.90	0.53
1:B:336:THR:HG21	1:B:392:ASN:HD21	1.73	0.53
1:D:164:ARG:NH1	1:D:539:ASP:OD1	2.39	0.53
1:C:277:ASN:HB3	1:C:280:LEU:HD12	1.89	0.53
1:E:92:TYR:CD2	1:E:92:TYR:N	2.75	0.53
1:C:180:VAL:HB	1:C:299:PHE:HA	1.89	0.53
1:F:486:ALA:O	1:F:490:GLN:HG3	2.08	0.53
1:A:128:HIS:ND1	1:A:133:ILE:HG13	2.24	0.53
1:C:357:GLN:NE2	1:C:532:THR:HG23	2.22	0.53
1:E:462:ARG:O	1:E:473:LEU:HD12	2.09	0.53
1:F:307:ASP:O	1:F:442:ARG:HB2	2.07	0.53
1:C:263:SER:HG	1:C:314:THR:HB	1.71	0.53
1:F:88:PRO:O	1:F:115:ARG:HB3	2.07	0.53
1:A:370:ALA:O	1:A:374:VAL:HG22	2.09	0.52
1:E:488:HIS:CE1	1:E:503:TRP:HE1	2.26	0.52
1:F:216:ARG:NH2	1:F:288:GLU:O	2.42	0.52
1:F:452:THR:HB	1:F:502:THR:HG23	1.90	0.52
1:F:194:HIS:O	1:F:198:GLU:HG3	2.09	0.52
1:F:436:ALA:N	1:F:445:GLY:O	2.43	0.52
1:C:227:LEU:O	1:C:230:ALA:N	2.43	0.52
1:F:320:ASN:HD21	1:F:334:VAL:H	1.57	0.52
1:C:311:ASN:ND2	1:C:313:ASP:OD2	2.43	0.52
1:F:390:LEU:CD1	1:F:504:PHE:HB2	2.40	0.52
1:E:62:ILE:HD13	1:E:68:SER:HA	1.92	0.52
1:E:415:PRO:O	1:E:419:ILE:HG13	2.10	0.52
1:E:590:LYS:C	3:E:702:HOH:O	2.49	0.52
1:A:210:MET:HB2	1:B:209:ASP:OD1	2.09	0.52
1:F:571:GLY:O	1:F:577:GLN:NE2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ASP:CG	1:C:257:ARG:HH12	2.14	0.51
1:E:450:PHE:CE2	1:E:500:PRO:HB3	2.45	0.51
1:F:200:TRP:CZ2	1:F:587:PRO:HG3	2.45	0.51
1:F:220:LYS:HA	1:F:222:TYR:CE2	2.45	0.51
1:B:131:LYS:O	1:D:590:LYS:NZ	2.39	0.51
1:A:138:ILE:HD13	1:A:562:TYR:OH	2.10	0.51
1:B:113:THR:O	1:E:363:ARG:NH2	2.42	0.51
1:D:451:LEU:HD13	1:D:501:THR:CG2	2.41	0.51
1:A:125:LEU:HD11	1:A:137:SER:CB	2.39	0.51
1:C:365:TYR:HB2	1:C:521:MET:SD	2.50	0.51
1:E:125:LEU:CD1	1:E:137:SER:HB2	2.41	0.51
1:E:370:ALA:O	1:E:374:VAL:HG12	2.11	0.51
1:E:572:MET:HG3	1:F:552:CYS:O	2.11	0.51
1:B:388:ILE:HD11	1:B:521:MET:HB2	1.92	0.51
1:D:77:ARG:HB2	1:D:77:ARG:NH2	2.24	0.51
1:C:286:VAL:CG2	1:E:19:ARG:NE	2.73	0.51
1:B:46:ARG:HD3	1:B:50:GLY:O	2.11	0.51
1:B:572:MET:HG3	1:E:552:CYS:O	2.11	0.51
1:E:220:LYS:HA	1:E:222:TYR:CE2	2.44	0.51
1:B:474:GLN:HE22	1:B:525:GLY:N	2.09	0.51
1:D:266:MET:HE3	1:D:305:TRP:CZ2	2.45	0.51
1:D:342:ASN:O	1:D:346:MET:HG3	2.10	0.51
1:F:389:HIS:NE2	1:F:501:THR:HG23	2.26	0.51
1:F:401:SER:O	1:F:402:CYS:HB2	2.10	0.51
1:C:19:ARG:HD3	1:C:24:GLU:OE1	2.11	0.50
1:C:570:HIS:O	1:C:580:ARG:NH1	2.43	0.50
1:C:371:VAL:HG11	1:C:379:LEU:CD1	2.41	0.50
1:B:200:TRP:CZ2	1:B:587:PRO:HG3	2.47	0.50
1:F:42:SER:OG	1:F:53:ILE:O	2.30	0.50
1:F:224:GLU:OE1	1:F:283:LYS:NZ	2.41	0.50
1:C:286:VAL:HG23	1:E:19:ARG:HD2	1.94	0.50
1:E:267:ALA:HA	1:E:319:LEU:HD11	1.92	0.50
1:A:13:PRO:O	1:A:62:ILE:HD12	2.12	0.50
1:F:209:ASP:HB3	1:F:211:THR:HG22	1.93	0.50
1:C:178:LEU:HB3	1:C:297:ALA:HB2	1.93	0.50
1:D:33:MET:HE3	1:D:86:VAL:HB	1.93	0.50
1:D:486:ALA:O	1:D:490:GLN:HG3	2.12	0.50
1:A:563:ARG:HD3	1:A:567:TRP:CD1	2.47	0.50
1:F:390:LEU:HD11	1:F:504:PHE:CB	2.41	0.50
1:B:271:ARG:HG3	1:B:332:PHE:CZ	2.47	0.49
1:E:110:PHE:HE2	1:E:144:GLN:OE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ARG:NH2	1:B:453:GLU:OE2	2.45	0.49
1:F:141:HIS:ND1	1:F:154:ASP:OD2	2.36	0.49
1:F:300:GLN:HA	1:F:338:ASN:HB2	1.94	0.49
1:C:321:SER:O	1:C:329:ARG:NH1	2.37	0.49
1:D:321:SER:O	1:D:329:ARG:NH1	2.44	0.49
1:B:145:ASP:CG	1:E:373:ARG:HH22	2.14	0.49
1:D:507:ARG:NH1	1:D:555:ASN:O	2.44	0.49
1:E:90:TRP:CZ2	1:F:185:MET:HE2	2.47	0.49
1:A:573:ASP:O	1:A:577:GLN:HG2	2.13	0.49
1:F:416:HIS:HA	1:F:419:ILE:HD12	1.95	0.49
1:C:396:ALA:O	1:C:397:ALA:C	2.51	0.49
1:E:145:ASP:CG	1:F:494:ARG:NH2	2.66	0.49
1:D:198:GLU:HB3	1:D:590:LYS:HE2	1.95	0.49
1:E:361:ASP:OD1	1:E:528:HIS:NE2	2.45	0.49
1:C:227:LEU:HG	1:C:231:LEU:CD1	2.43	0.48
1:B:321:SER:O	1:B:329:ARG:NH1	2.46	0.48
1:D:361:ASP:HB2	1:D:391:ILE:O	2.13	0.48
1:E:15:ILE:HA	1:E:89:CYS:SG	2.54	0.48
1:A:83:THR:HG23	1:A:103:ARG:HD2	1.95	0.48
1:B:99:MET:HA	1:B:133:ILE:HD12	1.96	0.48
1:C:221:ILE:HG23	1:C:285:LEU:HD13	1.96	0.48
1:C:240:TYR:OH	1:C:260:LEU:HD11	2.13	0.48
1:E:6:LEU:HD12	1:E:6:LEU:H	1.79	0.48
1:C:265:LEU:O	1:C:269:CYS:SG	2.62	0.48
1:C:286:VAL:HG23	1:E:19:ARG:HE	1.76	0.48
1:D:474:GLN:HE22	1:D:525:GLY:N	2.12	0.48
1:E:200:TRP:CE2	1:E:587:PRO:HG3	2.49	0.48
1:E:352:LEU:HD11	1:E:543:LEU:HD22	1.96	0.48
1:B:488:HIS:CE1	1:B:503:TRP:HE1	2.32	0.48
1:C:267:ALA:HB2	1:C:315:ALA:HA	1.94	0.47
1:D:227:LEU:HD22	1:D:265:LEU:HD21	1.94	0.47
1:D:389:HIS:NE2	1:D:501:THR:OG1	2.43	0.47
1:E:118:ALA:HB2	1:E:139:TYR:HE1	1.79	0.47
1:A:321:SER:O	1:A:329:ARG:NH1	2.47	0.47
1:A:15:ILE:HD11	1:A:26:LEU:HB2	1.96	0.47
1:A:474:GLN:HE22	1:A:525:GLY:N	2.12	0.47
1:B:220:LYS:HA	1:B:222:TYR:CE2	2.49	0.47
1:C:208:VAL:HA	1:F:304:HIS:HE1	1.80	0.47
1:D:6:LEU:HD13	1:D:47:HIS:CD2	2.49	0.47
1:E:361:ASP:OD1	1:E:528:HIS:CD2	2.67	0.47
1:B:221:ILE:HG23	1:B:285:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:LYS:O	1:C:279:LYS:HD3	2.14	0.47
1:C:362:VAL:HG12	1:C:521:MET:CE	2.45	0.47
1:E:340:SER:O	1:E:344:VAL:HG23	2.15	0.47
1:F:361:ASP:HB2	1:F:391:ILE:O	2.15	0.47
1:F:421:GLN:O	1:F:421:GLN:HG3	2.14	0.47
1:A:222:TYR:CE1	1:A:265:LEU:HD21	2.49	0.47
1:A:483:LEU:HB3	1:A:487:MET:HE2	1.97	0.47
1:A:14:VAL:HG23	1:A:87:THR:HB	1.95	0.47
1:A:158:LYS:NZ	3:A:701:HOH:O	2.48	0.47
1:A:227:LEU:HD13	1:A:265:LEU:HG	1.97	0.47
1:B:14:VAL:CG1	1:B:87:THR:HB	2.43	0.47
1:B:393:SER:HA	1:B:499:TRP:CD2	2.49	0.47
1:C:192:VAL:HG11	1:C:205:VAL:HG11	1.97	0.47
1:C:304:HIS:CB	1:F:211:THR:HG23	2.44	0.47
1:D:172:MET:HG2	1:D:347:LEU:HD21	1.96	0.47
1:E:320:ASN:HA	1:E:332:PHE:O	2.13	0.47
1:F:5:SER:HB3	1:F:79:ASN:HD22	1.80	0.47
1:F:390:LEU:HD22	1:F:531:LEU:HD11	1.97	0.47
1:A:519:SER:O	1:A:523:ASN:ND2	2.47	0.47
1:B:13:PRO:HG2	1:B:61:CYS:HA	1.97	0.47
1:B:357:GLN:OE1	1:B:532:THR:OG1	2.25	0.47
1:F:296:ALA:HA	1:F:333:VAL:HG13	1.95	0.47
1:F:367:SER:O	1:F:371:VAL:HG23	2.14	0.47
1:B:575:GLU:OE2	1:F:572:MET:N	2.48	0.47
1:F:304:HIS:CD2	1:F:304:HIS:N	2.82	0.47
1:D:243:ASP:OD1	1:D:245:ASN:HB2	2.14	0.47
1:A:548:ARG:NH1	1:A:586:GLY:O	2.43	0.47
1:E:61:CYS:O	1:E:67:GLU:CD	2.53	0.47
1:E:266:MET:HE1	1:E:312:GLY:HA2	1.97	0.47
1:C:233:TRP:CZ2	1:C:428:LEU:HD11	2.50	0.46
1:D:215:ARG:HG3	1:D:219:GLN:HE21	1.78	0.46
1:D:242:GLU:OE1	1:D:242:GLU:N	2.43	0.46
1:D:209:ASP:OD2	1:E:210:MET:HG3	2.15	0.46
1:E:72:GLU:OE1	1:E:103:ARG:NH2	2.46	0.46
1:C:287:GLU:OE1	1:F:303:ARG:NH1	2.36	0.46
1:F:462:ARG:HE	1:F:526:ALA:HB3	1.80	0.46
1:A:590:LYS:NZ	1:F:131:LYS:O	2.45	0.46
1:C:286:VAL:CG2	1:E:19:ARG:HD2	2.45	0.46
1:F:81:GLY:O	1:F:104:PRO:HD2	2.15	0.46
1:C:217:ILE:HG23	1:C:265:LEU:HD22	1.97	0.46
1:C:245:ASN:HD21	1:C:438:HIS:N	2.10	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:LEU:O	1:C:347:LEU:HD12	2.16	0.46
1:F:295:ILE:HD12	1:F:347:LEU:HD11	1.98	0.46
1:C:185:MET:HE3	1:C:302:GLN:HB2	1.98	0.46
1:F:573:ASP:O	1:F:577:GLN:HG2	2.15	0.46
1:A:88:PRO:O	1:A:115:ARG:HB3	2.16	0.46
1:C:175:LYS:O	1:C:203:MET:HG2	2.16	0.46
1:C:210:MET:HB2	1:F:209:ASP:OD1	2.16	0.46
1:E:303:ARG:NH2	1:E:307:ASP:OD2	2.49	0.46
1:F:499:TRP:HB3	1:F:500:PRO:HD2	1.98	0.46
1:C:49:CYS:C	1:C:416:HIS:HE2	2.19	0.46
1:F:5:SER:HB3	1:F:79:ASN:ND2	2.31	0.46
1:F:209:ASP:OD1	1:F:211:THR:HG22	2.16	0.46
1:F:377:GLN:HE22	1:F:486:ALA:CB	2.27	0.46
1:F:6:LEU:HD13	1:F:47:HIS:CD2	2.51	0.46
1:A:442:ARG:CZ	1:D:20:MET:HE3	2.46	0.45
1:A:588:LEU:HB3	1:A:589:TYR:CD2	2.50	0.45
1:C:300:GLN:HA	1:C:338:ASN:HB2	1.98	0.45
1:A:133:ILE:HG13	1:A:133:ILE:O	2.16	0.45
1:F:336:THR:HG21	1:F:392:ASN:ND2	2.30	0.45
1:B:75:PHE:CD2	1:B:80:VAL:HG21	2.51	0.45
1:E:524:TRP:HD1	1:E:526:ALA:O	2.00	0.45
1:D:224:GLU:HG3	1:D:283:LYS:HZ2	1.80	0.45
1:A:92:TYR:N	1:A:92:TYR:CD1	2.82	0.45
1:A:283:LYS:O	1:A:283:LYS:HG2	2.16	0.45
1:A:309:TYR:HB3	1:A:310:PRO:CD	2.46	0.45
1:D:264:LEU:O	1:D:268:MET:HG3	2.16	0.45
1:E:371:VAL:HG11	1:E:379:LEU:HG	1.97	0.45
1:B:454:GLY:HA3	1:B:482:GLU:HB2	1.98	0.45
1:C:239:ARG:HD3	1:C:239:ARG:N	2.31	0.45
1:C:513:PRO:O	1:C:519:SER:HB2	2.15	0.45
1:F:420:SER:O	1:F:423:GLU:HB2	2.17	0.45
1:A:18:ARG:HG3	1:A:22:VAL:CG1	2.47	0.45
1:E:113:THR:OG1	1:F:494:ARG:HG2	2.17	0.45
1:A:346:MET:CE	1:A:359:PHE:HD2	2.28	0.45
1:B:519:SER:HA	1:B:522:ALA:HB3	1.99	0.45
1:E:105:LYS:HE2	1:E:133:ILE:CG2	2.47	0.45
1:E:460:MET:HA	1:E:530:VAL:O	2.17	0.45
1:F:92:TYR:N	1:F:92:TYR:CD1	2.81	0.45
1:A:8:LYS:CG	1:A:54:GLU:HB2	2.47	0.45
1:B:438:HIS:CD2	1:B:442:ARG:HA	2.52	0.45
1:E:92:TYR:OH	1:F:303:ARG:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:VAL:HG12	1:A:75:PHE:CE1	2.52	0.44
1:D:33:MET:HE2	1:D:86:VAL:HB	1.98	0.44
1:F:9:ILE:HD12	1:F:41:ILE:HD13	1.99	0.44
1:B:157:GLU:OE2	1:B:560:LYS:NZ	2.50	0.44
1:F:358:VAL:HB	1:F:531:LEU:HB2	1.99	0.44
1:C:383:ALA:O	1:C:384:GLU:C	2.55	0.44
1:E:31:MET:HG3	1:E:61:CYS:SG	2.58	0.44
1:A:480:SER:HA	1:A:503:TRP:O	2.17	0.44
1:B:563:ARG:NH2	1:B:578:ASP:OD2	2.50	0.44
1:E:243:ASP:HB3	1:E:250:LYS:CE	2.48	0.44
1:E:387:ILE:HD12	1:E:387:ILE:HA	1.88	0.44
1:A:513:PRO:HG2	1:D:572:MET:HG2	1.99	0.44
1:C:358:VAL:HB	1:C:531:LEU:HB2	1.98	0.44
1:D:221:ILE:O	1:D:221:ILE:HG22	2.18	0.44
1:C:563:ARG:HD3	1:C:567:TRP:CD1	2.52	0.44
1:E:168:ALA:O	1:E:172:MET:HG3	2.17	0.44
1:E:458:PHE:HB3	1:E:531:LEU:HD22	2.00	0.44
1:C:215:ARG:NH1	1:C:221:ILE:HD11	2.32	0.44
1:C:286:VAL:CG2	1:E:19:ARG:CD	2.95	0.44
1:D:483:LEU:HD22	1:D:487:MET:HE2	2.00	0.44
1:F:12:ARG:HB2	1:F:85:THR:HA	2.00	0.44
1:B:130:GLN:O	1:E:467:LYS:HB2	2.17	0.44
1:B:364:THR:HG21	1:F:113:THR:HG22	2.00	0.44
1:B:379:LEU:HD22	1:B:383:ALA:HB1	2.00	0.44
1:D:220:LYS:HA	1:D:222:TYR:CE2	2.53	0.44
1:D:432:GLU:OE1	1:D:449:ARG:NH2	2.36	0.44
1:C:164:ARG:NH1	1:C:539:ASP:OD1	2.49	0.44
1:C:252:ASP:HB3	1:C:255:GLN:H	1.82	0.44
1:C:389:HIS:HB2	1:C:503:TRP:CZ3	2.53	0.44
1:E:517:VAL:O	1:E:520:VAL:HB	2.18	0.43
1:E:577:GLN:HG3	1:E:578:ASP:N	2.32	0.43
1:F:477:GLU:OE2	1:F:507:ARG:NH2	2.51	0.43
1:A:9:ILE:HD12	1:A:41:ILE:HG21	2.00	0.43
1:D:391:ILE:HD11	1:D:499:TRP:HB2	2.01	0.43
1:B:348:MET:HG2	1:B:543:LEU:HD21	2.01	0.43
1:C:475:ILE:O	1:C:554:HIS:HA	2.18	0.43
1:A:363:ARG:HD2	1:D:119:VAL:HG21	2.00	0.43
1:C:466:ILE:HG21	1:C:469:LEU:HD23	2.01	0.43
1:C:487:MET:HE2	1:C:487:MET:HB3	1.89	0.43
1:A:57:ILE:HG22	1:A:58:ALA:N	2.34	0.43
1:F:288:GLU:OE1	1:F:288:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLY:HA3	1:C:467:LYS:HD3	2.00	0.43
1:E:19:ARG:HB3	1:E:20:MET:H	1.70	0.43
1:E:266:MET:CE	1:E:312:GLY:HA2	2.49	0.43
1:F:437:ILE:HD11	1:F:498:THR:HG21	1.99	0.43
1:F:485:LYS:O	1:F:489:ASP:OD1	2.37	0.43
1:C:320:ASN:HD21	1:C:334:VAL:H	1.65	0.43
1:B:292:TYR:O	1:B:293:ASN:C	2.57	0.43
1:D:345:ALA:HB3	1:D:530:VAL:HG21	2.00	0.43
1:F:10:GLY:HA2	1:F:56:VAL:O	2.19	0.43
1:F:127:ALA:O	1:F:131:LYS:HG3	2.19	0.43
1:F:303:ARG:NH2	1:F:307:ASP:OD2	2.51	0.43
1:B:513:PRO:HG3	1:F:572:MET:HG2	2.01	0.43
1:C:314:THR:HG23	1:C:433:TRP:HZ3	1.82	0.43
1:D:269:CYS:O	1:D:273:MET:HG3	2.17	0.43
1:F:99:MET:HA	1:F:133:ILE:HD12	2.01	0.43
1:F:246:ALA:HB1	1:F:248:HIS:CE1	2.53	0.43
1:A:8:LYS:O	1:A:80:VAL:HA	2.18	0.43
1:A:18:ARG:NH2	1:C:302:GLN:OE1	2.46	0.43
1:B:265:LEU:HD23	1:B:265:LEU:HA	1.84	0.43
1:E:37:THR:O	1:E:41:ILE:HG13	2.18	0.43
1:A:121:LEU:O	1:A:125:LEU:HG	2.19	0.42
1:D:226:GLU:HB3	1:D:268:MET:CE	2.48	0.42
1:D:460:MET:HA	1:D:530:VAL:O	2.19	0.42
1:E:15:ILE:HD11	1:E:26:LEU:HB2	2.01	0.42
1:E:243:ASP:HB3	1:E:250:LYS:HE3	1.99	0.42
1:E:474:GLN:HG2	1:E:552:CYS:SG	2.59	0.42
1:A:206:GLN:HG2	1:A:292:TYR:CD1	2.54	0.42
1:B:152:PRO:HB2	1:B:154:ASP:OD1	2.20	0.42
1:C:208:VAL:HA	1:F:304:HIS:CE1	2.54	0.42
1:F:302:GLN:HG2	1:F:306:THR:HG21	2.01	0.42
1:F:341:LEU:HB2	1:F:462:ARG:NH1	2.33	0.42
1:B:222:TYR:CD1	1:B:265:LEU:CD2	3.01	0.42
1:B:406:ASP:OD1	1:B:410:LYS:N	2.52	0.42
1:C:452:THR:HB	1:C:502:THR:HG23	2.00	0.42
1:A:209:ASP:OD1	1:B:210:MET:HB2	2.19	0.42
1:A:423:GLU:O	1:A:426:ALA:HB3	2.20	0.42
1:F:313:ASP:HB3	1:F:447:SER:HA	2.01	0.42
1:A:234:ALA:O	1:A:238:PHE:HB2	2.20	0.42
1:B:158:LYS:O	1:B:159:LEU:C	2.56	0.42
1:B:329:ARG:NH1	1:B:331:PRO:HA	2.33	0.42
1:C:19:ARG:O	1:C:20:MET:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:GLY:HA2	1:C:417:TRP:CE3	2.54	0.42
1:C:259:VAL:HG22	1:C:310:PRO:HG3	2.02	0.42
1:E:31:MET:O	1:E:35:LYS:HG3	2.19	0.42
1:F:164:ARG:HD3	1:F:352:LEU:O	2.20	0.42
1:F:390:LEU:N	1:F:390:LEU:HD12	2.35	0.42
1:E:22:VAL:O	1:E:25:SER:OG	2.38	0.42
1:E:118:ALA:HB2	1:E:139:TYR:CE1	2.55	0.42
1:B:536:VAL:HG23	1:B:540:PHE:HD2	1.85	0.42
1:C:90:TRP:HE1	1:D:185:MET:CE	2.33	0.42
1:C:285:LEU:HD22	1:C:288:GLU:OE2	2.20	0.42
1:D:387:ILE:HD11	1:D:481:VAL:HG21	2.02	0.42
1:E:315:ALA:O	1:E:319:LEU:HD12	2.20	0.42
1:F:352:LEU:HD13	1:F:539:ASP:HB3	2.02	0.42
1:A:11:ILE:CD1	1:A:55:CYS:HB3	2.50	0.42
1:B:267:ALA:HB2	1:B:315:ALA:HA	2.02	0.42
1:C:405:ARG:HB3	1:C:409:GLY:HA2	2.02	0.42
1:E:263:SER:HB3	1:E:314:THR:HB	2.01	0.42
1:F:252:ASP:OD1	1:F:252:ASP:N	2.28	0.42
1:F:345:ALA:HB3	1:F:530:VAL:HG21	2.01	0.42
1:B:310:PRO:HA	1:B:444:GLY:O	2.19	0.42
1:C:488:HIS:ND1	1:C:488:HIS:C	2.74	0.42
1:F:75:PHE:HB3	1:F:80:VAL:HG22	2.02	0.42
1:D:314:THR:HG23	1:D:433:TRP:CZ3	2.55	0.41
1:F:268:MET:HG3	1:F:325:TRP:HZ2	1.84	0.41
1:F:270:ILE:O	1:F:274:MET:HG3	2.20	0.41
1:F:366:TRP:CZ3	1:F:374:VAL:HG21	2.55	0.41
1:F:370:ALA:O	1:F:374:VAL:HG22	2.20	0.41
1:F:527:ASN:OD1	1:F:527:ASN:N	2.52	0.41
1:C:216:ARG:HH12	1:C:272:ASP:HB2	1.85	0.41
1:C:362:VAL:HG12	1:C:521:MET:HE3	2.02	0.41
1:D:412:THR:OG1	1:D:413:MET:N	2.52	0.41
1:F:302:GLN:HA	1:F:303:ARG:HA	1.88	0.41
1:A:212:GLU:HB2	1:B:304:HIS:CD2	2.56	0.41
1:A:286:VAL:HG23	1:F:19:ARG:NE	2.36	0.41
1:D:485:LYS:HA	1:D:485:LYS:HD3	1.91	0.41
1:D:573:ASP:OD2	1:D:576:GLY:N	2.47	0.41
1:E:387:ILE:HD11	1:E:481:VAL:CG2	2.50	0.41
1:E:462:ARG:NH1	1:E:528:HIS:HB2	2.35	0.41
1:B:318:LEU:O	1:B:329:ARG:NH2	2.50	0.41
1:C:483:LEU:HD13	1:C:487:MET:HE2	2.02	0.41
1:D:183:VAL:HA	1:D:190:SER:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:THR:HB	1:E:502:THR:HB	2.02	0.41
1:F:388:ILE:O	1:F:390:LEU:HD12	2.20	0.41
1:C:16:ASP:O	1:C:23:ARG:HG3	2.19	0.41
1:C:392:ASN:ND2	1:C:395:SER:O	2.51	0.41
1:D:183:VAL:HA	1:D:190:SER:HB3	2.03	0.41
1:D:395:SER:O	1:D:396:ALA:HB2	2.20	0.41
1:A:216:ARG:CZ	1:A:273:MET:HG2	2.51	0.41
1:D:124:ALA:O	1:D:127:ALA:HB3	2.20	0.41
1:E:136:PHE:CE2	1:E:542:THR:HG23	2.56	0.41
1:E:572:MET:N	1:F:575:GLU:OE1	2.54	0.41
1:F:59:ASP:OD1	1:F:74:LYS:NZ	2.44	0.41
1:B:383:ALA:CB	1:B:387:ILE:HD13	2.50	0.41
1:C:9:ILE:HD12	1:C:41:ILE:HG21	2.03	0.41
1:E:213:LEU:HD21	1:E:266:MET:HG2	2.02	0.41
1:F:193:ASP:HB3	1:F:196:PHE:HB3	2.03	0.41
1:F:516:ASP:OD1	1:F:518:TYR:N	2.54	0.41
1:A:94:SER:HB3	1:C:186:GLY:CA	2.51	0.41
1:D:304:HIS:NE2	1:E:208:VAL:HG13	2.36	0.41
1:E:145:ASP:CG	1:F:373:ARG:NH2	2.74	0.41
1:F:319:LEU:O	1:F:332:PHE:HB2	2.20	0.41
1:A:56:VAL:HG12	1:A:75:PHE:HE1	1.86	0.41
1:C:108:TRP:CD1	1:C:138:ILE:HG22	2.56	0.41
1:C:304:HIS:HB2	1:F:211:THR:HG23	2.03	0.41
1:D:118:ALA:CB	1:D:139:TYR:CE1	3.04	0.41
1:E:92:TYR:N	1:E:92:TYR:HD2	2.15	0.41
1:E:391:ILE:HD11	1:E:499:TRP:HB2	2.03	0.41
1:F:236:LYS:HE3	1:F:237:ASN:OD1	2.21	0.41
1:F:240:TYR:C	1:F:432:GLU:HG2	2.41	0.41
1:B:204:LYS:HE2	1:D:99:MET:HG3	2.02	0.41
1:B:243:ASP:OD1	1:B:245:ASN:HB2	2.20	0.41
1:E:450:PHE:CD2	1:E:500:PRO:HB3	2.55	0.41
1:F:374:VAL:O	1:F:490:GLN:OE1	2.39	0.41
1:E:40:LEU:O	1:E:44:LYS:HG2	2.22	0.40
1:A:151:ILE:HA	1:A:152:PRO:HD3	1.88	0.40
1:A:474:GLN:HE22	1:A:524:TRP:HA	1.86	0.40
1:B:358:VAL:HB	1:B:531:LEU:HB2	2.03	0.40
1:D:87:THR:HG21	1:D:120:TYR:CD2	2.56	0.40
1:D:271:ARG:HG3	1:D:332:PHE:CZ	2.55	0.40
1:D:308:GLN:NE2	1:E:215:ARG:HB2	2.36	0.40
1:E:233:TRP:CD1	1:E:325:TRP:HA	2.56	0.40
1:E:427:CYS:O	1:E:431:THR:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:ARG:HD3	1:B:567:TRP:CD1	2.56	0.40
1:E:165:ALA:HA	1:E:352:LEU:HD21	2.03	0.40
1:E:359:PHE:HD1	1:E:392:ASN:HD21	1.68	0.40
1:A:359:PHE:O	1:A:392:ASN:HB2	2.21	0.40
1:C:313:ASP:HA	1:C:395:SER:HB3	2.03	0.40
1:E:90:TRP:HZ2	1:F:185:MET:HB3	1.86	0.40
1:E:260:LEU:HD13	1:E:264:LEU:HD12	2.03	0.40
1:C:304:HIS:HB3	1:F:211:THR:HG23	2.02	0.40
1:C:319:LEU:O	1:C:332:PHE:HB2	2.22	0.40
1:E:264:LEU:O	1:E:268:MET:HG3	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:THR:OG1	1:F:59:ASP:OD2[4_545]	2.09	0.11
1:A:377:GLN:OE1	1:F:78:GLN:NE2[4_545]	2.17	0.03
1:C:282:GLU:OE1	1:D:77:ARG:NH2[2_545]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	584/612 (95%)	556 (95%)	24 (4%)	4 (1%)	22	56
1	B	584/612 (95%)	553 (95%)	29 (5%)	2 (0%)	41	73
1	C	584/612 (95%)	540 (92%)	38 (6%)	6 (1%)	15	48
1	D	584/612 (95%)	562 (96%)	21 (4%)	1 (0%)	47	79
1	E	584/612 (95%)	552 (94%)	26 (4%)	6 (1%)	15	48
1	F	584/612 (95%)	550 (94%)	27 (5%)	7 (1%)	13	43
All	All	3504/3672 (95%)	3313 (94%)	165 (5%)	26 (1%)	22	56

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	495	THR
1	A	283	LYS
1	B	93	GLY
1	C	384	GLU
1	F	47	HIS
1	F	93	GLY
1	F	393	SER
1	A	88	PRO
1	A	495	THR
1	C	397	ALA
1	E	495	THR
1	D	88	PRO
1	F	495	THR
1	E	245	ASN
1	F	346	MET
1	C	283	LYS
1	E	13	PRO
1	F	88	PRO
1	F	378	PRO
1	C	88	PRO
1	C	391	ILE
1	E	116	PRO
1	A	378	PRO
1	B	88	PRO
1	E	88	PRO
1	E	561	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	466/489 (95%)	452 (97%)	14 (3%)	41	72
1	B	466/489 (95%)	455 (98%)	11 (2%)	49	77
1	C	466/489 (95%)	457 (98%)	9 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	466/489 (95%)	455 (98%)	11 (2%)	49	77
1	E	466/489 (95%)	446 (96%)	20 (4%)	29	62
1	F	466/489 (95%)	450 (97%)	16 (3%)	37	69
All	All	2796/2934 (95%)	2715 (97%)	81 (3%)	42	73

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	31	MET
1	A	94	SER
1	A	137	SER
1	A	145	ASP
1	A	156	GLU
1	A	194	HIS
1	A	329	ARG
1	A	336	THR
1	A	399	ASP
1	A	482	GLU
1	A	494	ARG
1	A	498	THR
1	A	567	TRP
1	B	14	VAL
1	B	31	MET
1	B	49	CYS
1	B	194	HIS
1	B	251	ARG
1	B	257	ARG
1	B	336	THR
1	B	447	SER
1	B	497	SER
1	B	521	MET
1	B	548	ARG
1	C	6	LEU
1	C	73	GLU
1	C	239	ARG
1	C	286	VAL
1	C	361	ASP
1	C	420	SER
1	C	496	ASN
1	C	567	TRP

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Mol	Chain	Res	Type
1	C	587	PRO
1	D	115	ARG
1	D	179	SER
1	D	214	ARG
1	D	263	SER
1	D	329	ARG
1	D	342	ASN
1	D	361	ASP
1	D	393	SER
1	D	395	SER
1	D	422	LYS
1	D	501	THR
1	E	18	ARG
1	E	29	GLN
1	E	31	MET
1	E	68	SER
1	E	91	CYS
1	E	94	SER
1	E	164	ARG
1	E	214	ARG
1	E	251	ARG
1	E	252	ASP
1	E	262	GLU
1	E	322	SER
1	E	367	SER
1	E	373	ARG
1	E	395	SER
1	E	420	SER
1	E	431	THR
1	E	467	LYS
1	E	485	LYS
1	E	502	THR
1	F	5	SER
1	F	49	CYS
1	F	52	GLN
1	F	94	SER
1	F	190	SER
1	F	214	ARG
1	F	227	LEU
1	F	279	LYS
1	F	361	ASP
1	F	363	ARG

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Mol	Chain	Res	Type
1	F	364	THR
1	F	403	GLN
1	F	405	ARG
1	F	428	LEU
1	F	462	ARG
1	F	498	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	GLN
1	B	438	HIS
1	B	474	GLN
1	B	488	HIS
1	C	245	ASN
1	C	496	ASN
1	D	219	GLN
1	E	244	GLN
1	E	404	GLN
1	F	144	GLN
1	F	293	ASN
1	F	320	ASN
1	F	377	GLN
1	F	404	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	586/612 (95%)	-0.28	6 (1%)	82	68	28, 52, 76, 96	0
1	B	586/612 (95%)	-0.19	12 (2%)	65	48	29, 58, 85, 107	0
1	C	586/612 (95%)	-0.04	21 (3%)	42	28	30, 61, 89, 111	0
1	D	586/612 (95%)	-0.35	3 (0%)	91	81	27, 48, 72, 100	0
1	E	586/612 (95%)	0.08	21 (3%)	42	28	36, 67, 92, 118	0
1	F	586/612 (95%)	0.11	23 (3%)	39	25	33, 71, 101, 127	0
All	All	3516/3672 (95%)	-0.11	86 (2%)	59	42	27, 59, 90, 127	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	382	LEU	5.0
1	C	252	ASP	4.7
1	F	249	TYR	4.4
1	C	251	ARG	4.3
1	C	246	ALA	4.2
1	E	407	GLU	4.0
1	F	407	GLU	4.0
1	E	147	ASP	4.0
1	F	417	TRP	3.9
1	C	407	GLU	3.8
1	C	249	TYR	3.8
1	F	253	GLU	3.7
1	E	249	TYR	3.5
1	E	248	HIS	3.4
1	F	282	GLU	3.4
1	B	242	GLU	3.2
1	D	407	GLU	3.2
1	B	248	HIS	3.1
1	F	247	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	246	ALA	3.0
1	C	242	GLU	3.0
1	C	247	GLN	2.9
1	A	407	GLU	2.9
1	C	455	GLY	2.9
1	C	256	SER	2.9
1	B	371	VAL	2.8
1	E	410	LYS	2.8
1	E	420	SER	2.8
1	B	147	ASP	2.8
1	F	52	GLN	2.8
1	F	254	GLU	2.8
1	F	406	ASP	2.8
1	F	242	GLU	2.8
1	F	511	LYS	2.8
1	C	317	ALA	2.7
1	C	509	THR	2.7
1	F	374	VAL	2.7
1	C	254	GLU	2.6
1	A	247	GLN	2.6
1	E	45	LEU	2.6
1	E	282	GLU	2.5
1	F	408	GLU	2.5
1	B	407	GLU	2.5
1	E	254	GLU	2.5
1	A	278	GLU	2.5
1	C	253	GLU	2.5
1	E	242	GLU	2.4
1	E	417	TRP	2.4
1	F	409	GLY	2.4
1	F	285	LEU	2.3
1	E	247	GLN	2.3
1	F	248	HIS	2.3
1	D	243	ASP	2.3
1	C	220	LYS	2.3
1	B	377	GLN	2.3
1	E	382	LEU	2.2
1	B	20	MET	2.2
1	D	410	LYS	2.2
1	B	21	GLY	2.2
1	F	50	GLY	2.2
1	E	240	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	403	GLN	2.2
1	C	255	GLN	2.1
1	C	315	ALA	2.1
1	F	380	THR	2.1
1	F	255	GLN	2.1
1	F	427	CYS	2.1
1	C	385	HIS	2.1
1	E	150	THR	2.1
1	B	249	TYR	2.1
1	A	147	ASP	2.1
1	A	282	GLU	2.1
1	E	402	CYS	2.1
1	C	285	LEU	2.1
1	E	239	ARG	2.1
1	E	146	ALA	2.0
1	E	411	PRO	2.0
1	F	147	ASP	2.0
1	E	486	ALA	2.0
1	C	243	ASP	2.0
1	E	52	GLN	2.0
1	A	21	GLY	2.0
1	B	243	ASP	2.0
1	C	282	GLU	2.0
1	C	284	GLY	2.0
1	B	417	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	MN	F	601	1/1	0.77	0.15	90,90,90,90	0
2	MN	E	601	1/1	0.85	0.20	81,81,81,81	0
2	MN	D	601	1/1	0.85	0.16	73,73,73,73	0
2	MN	B	601	1/1	0.86	0.20	64,64,64,64	0
2	MN	C	601	1/1	0.93	0.23	74,74,74,74	0
2	MN	A	601	1/1	0.94	0.14	69,69,69,69	0

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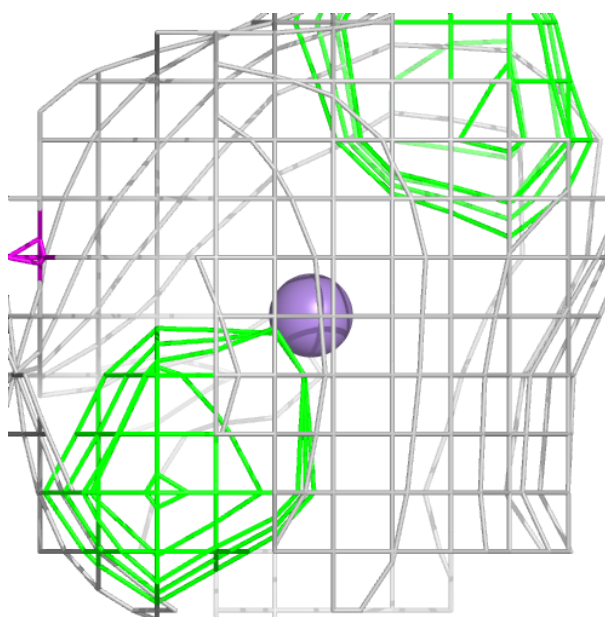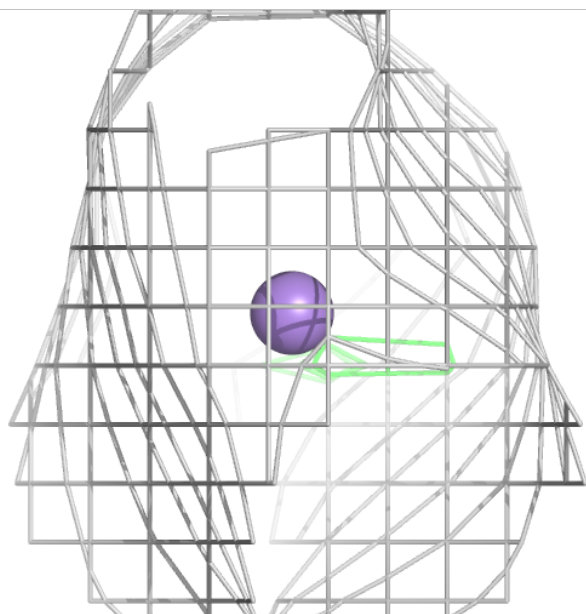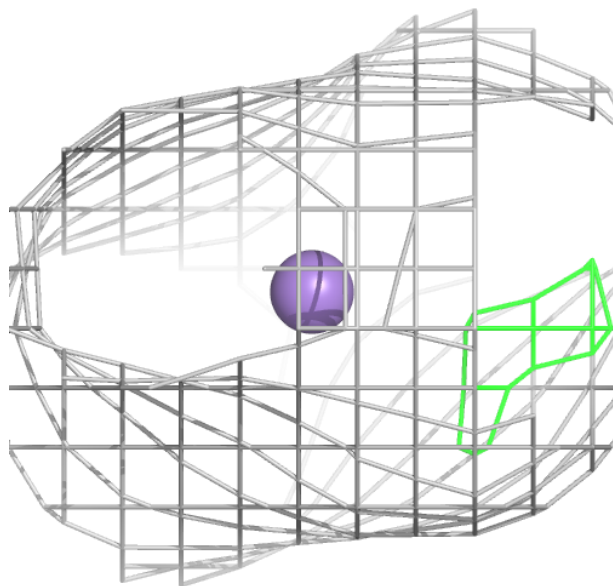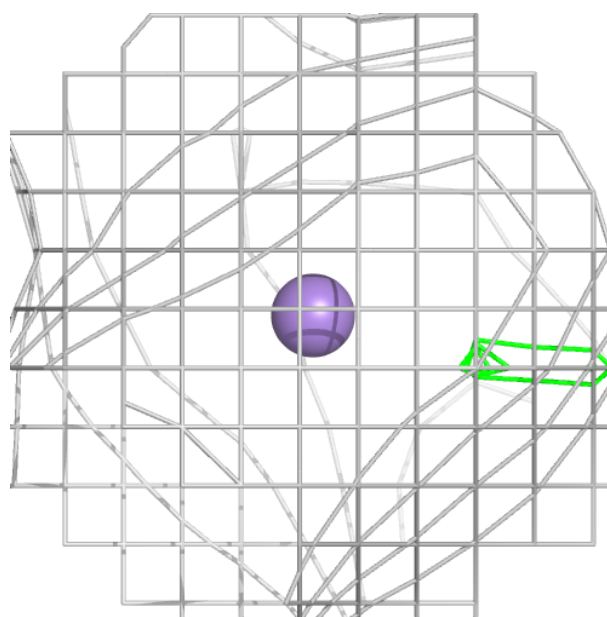

Electron density around MN F 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
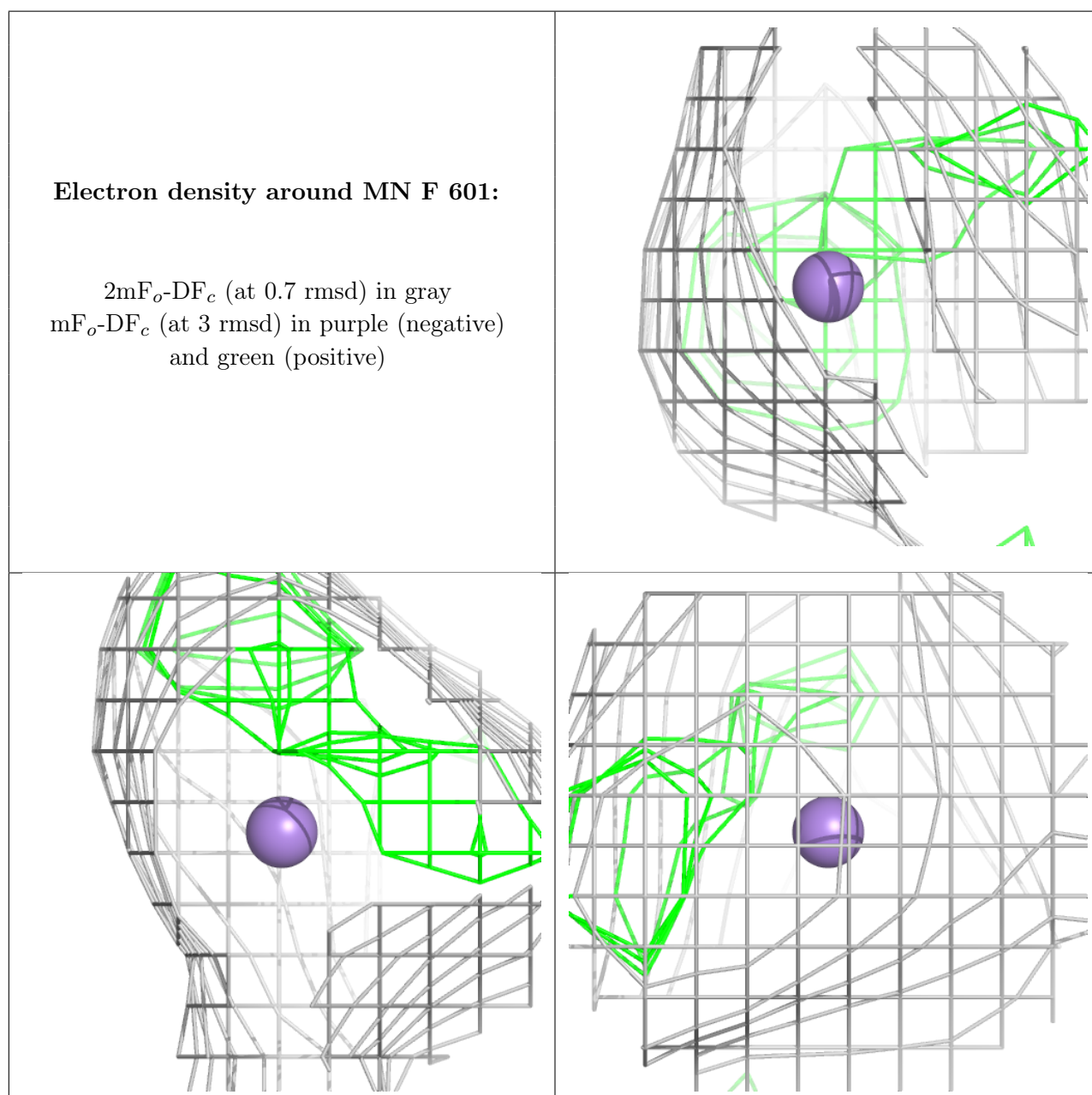
Electron density around MN E 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
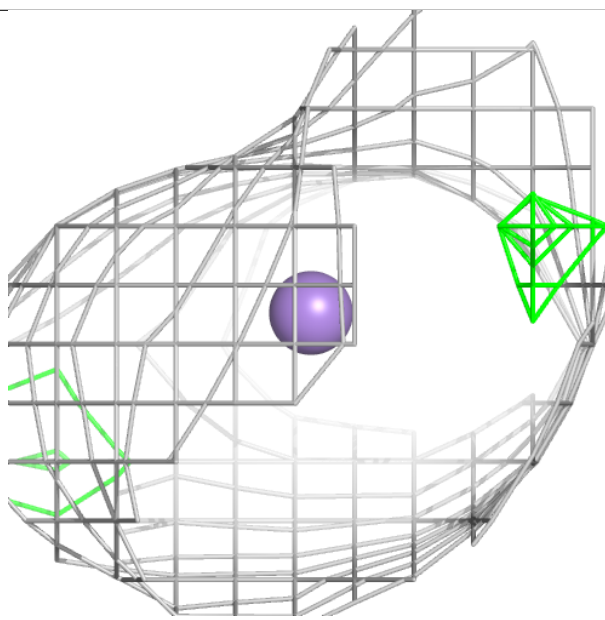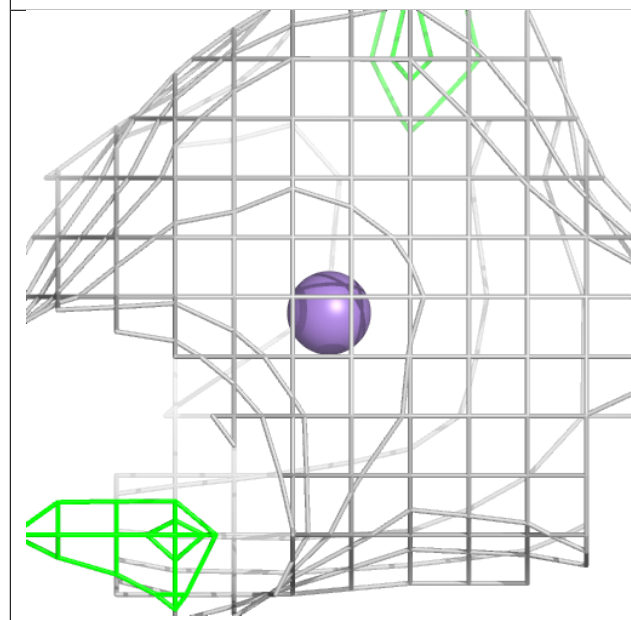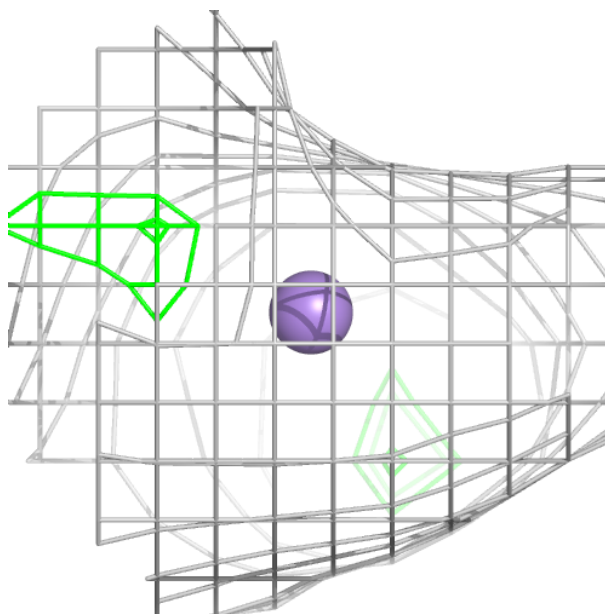
Electron density around MN D 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
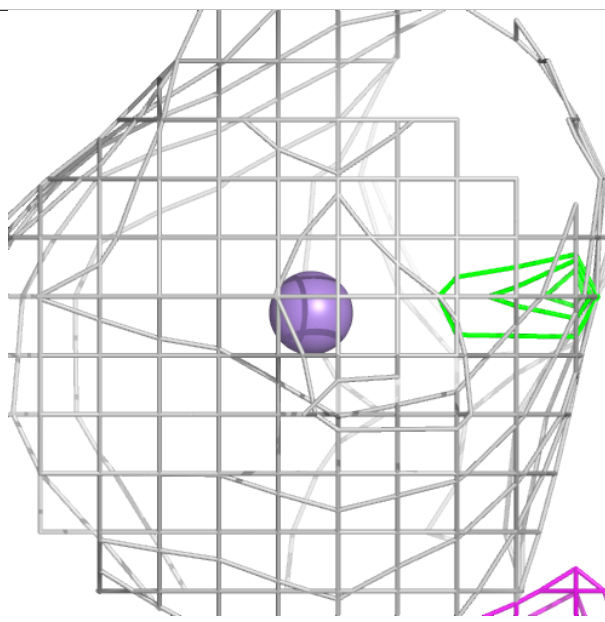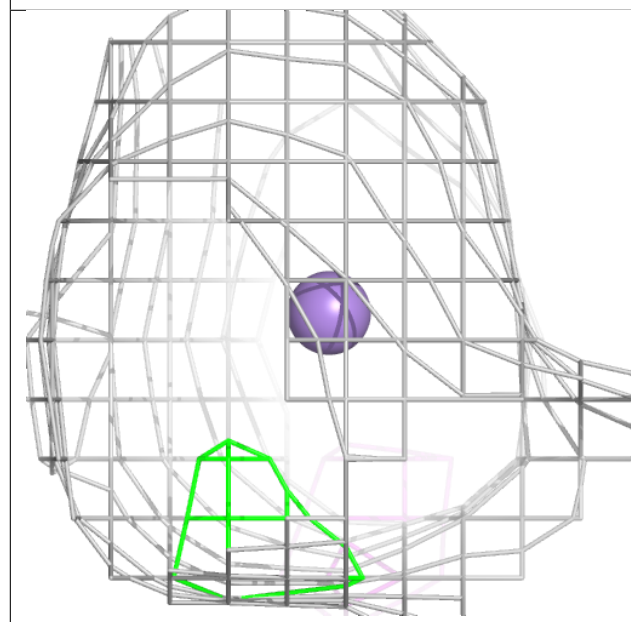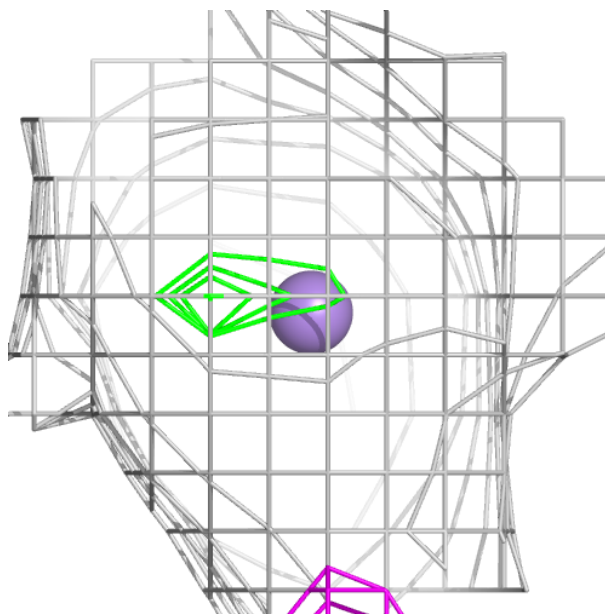
Electron density around MN B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
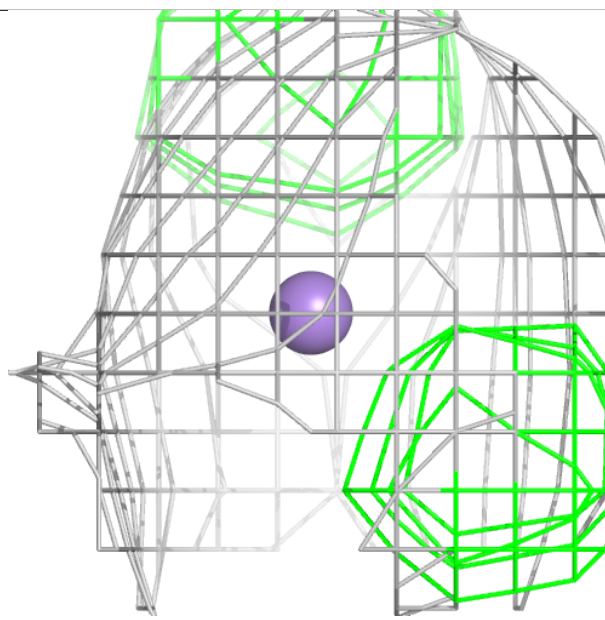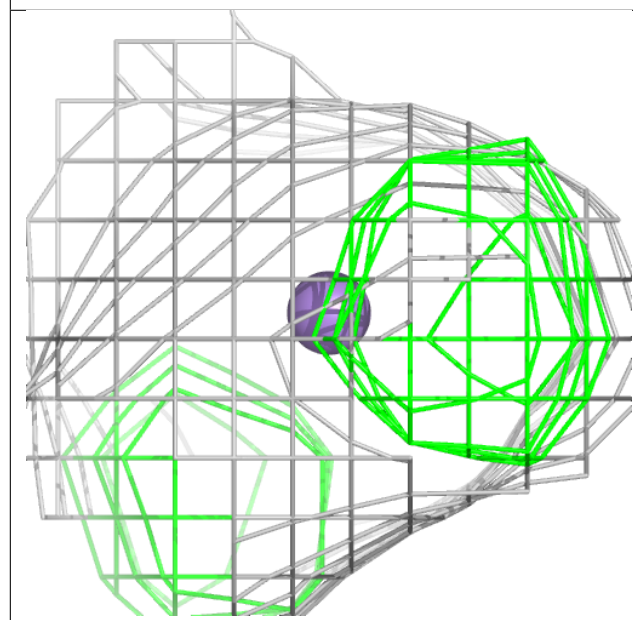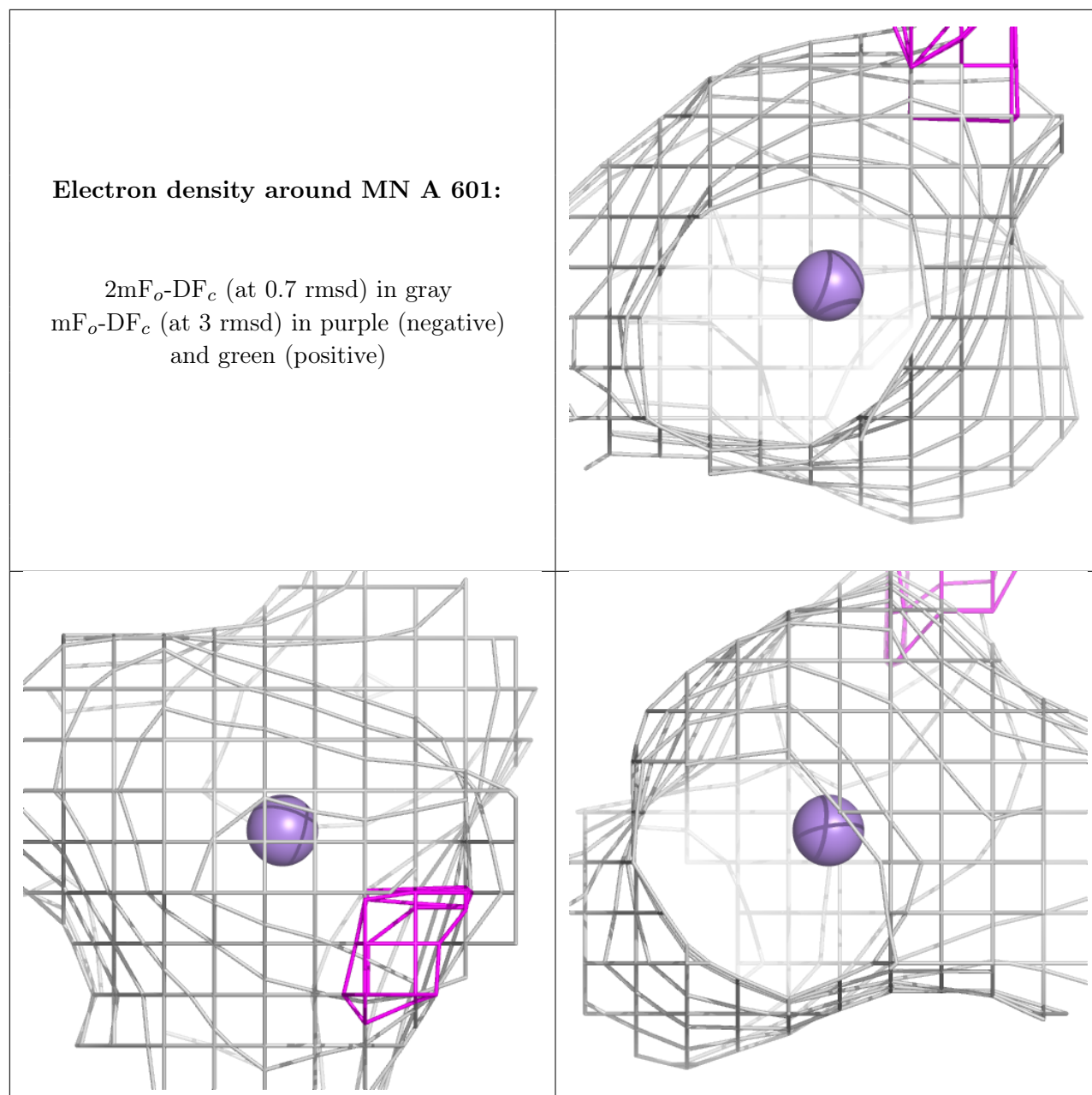
Electron density around MN C 601:

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

Electron density around MN A 601:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.