



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:25 AM UTC

PDB ID : 6K1G / pdb_00006k1g
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)

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
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

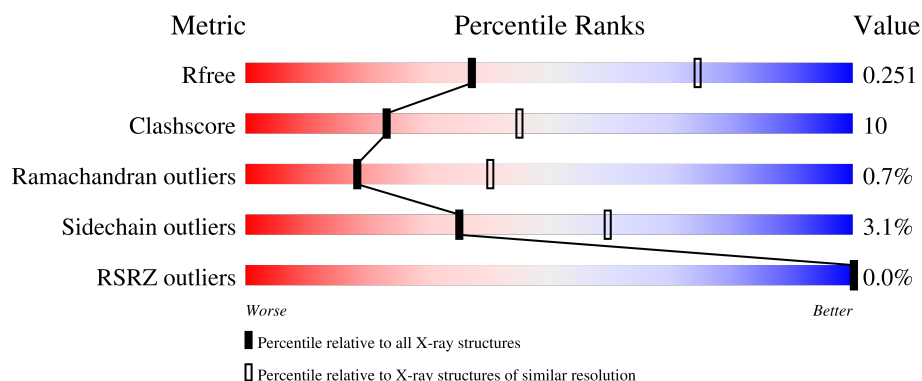
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

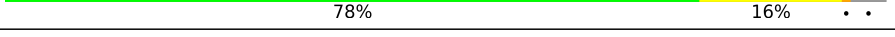
The reported resolution of this entry is 2.96 Å.

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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	612	 76%19% . .
1	B	612	 76%19% . .
1	C	612	 69%25% . .
1	D	612	 78%16% . .
1	E	612	 69%24% . .

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Mol	Chain	Length	Quality of chain
1	F	612	65% 29% . .

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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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 (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

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

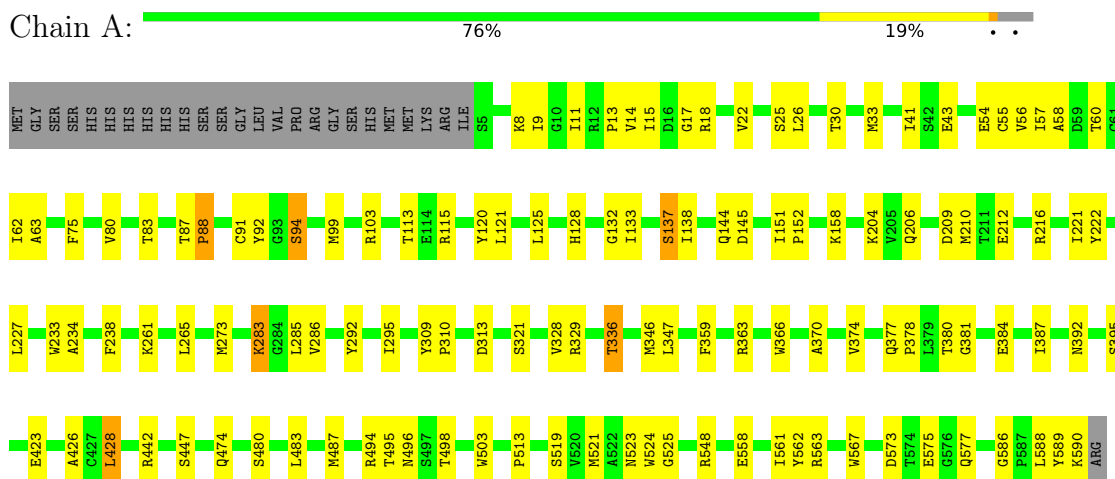
- Molecule 3 is water.

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

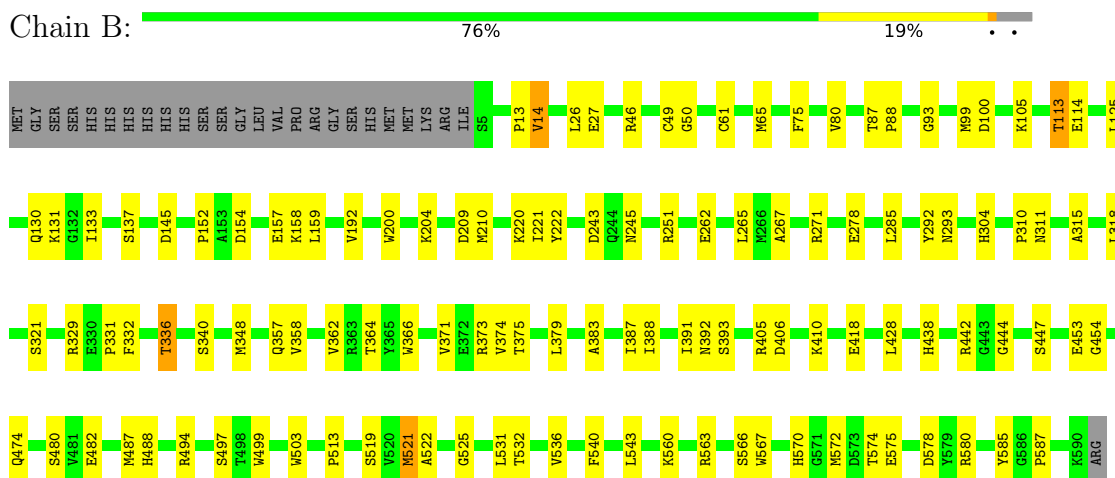
3 Residue-property plots

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.

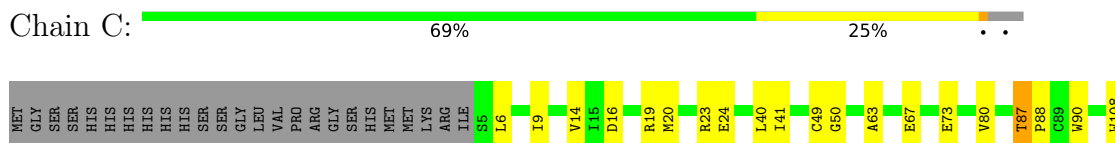
• Molecule 1: L-fucose isomerase

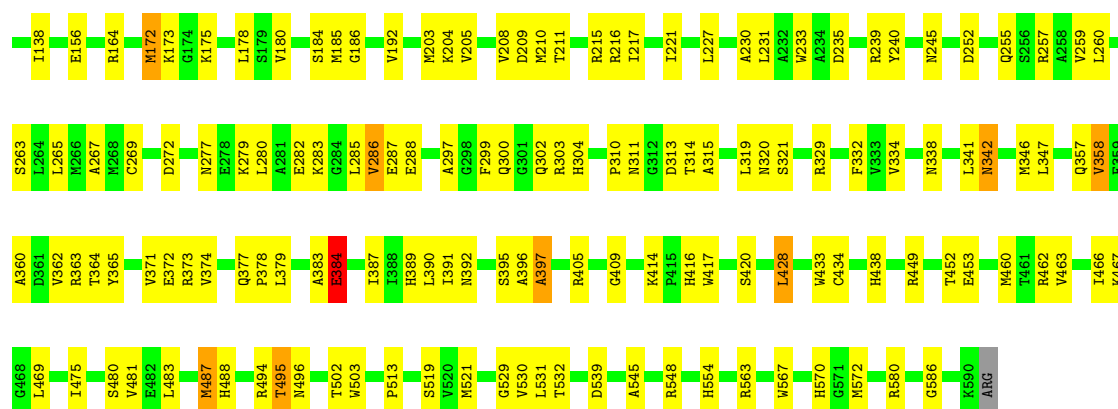


• Molecule 1: L-fucose isomerase



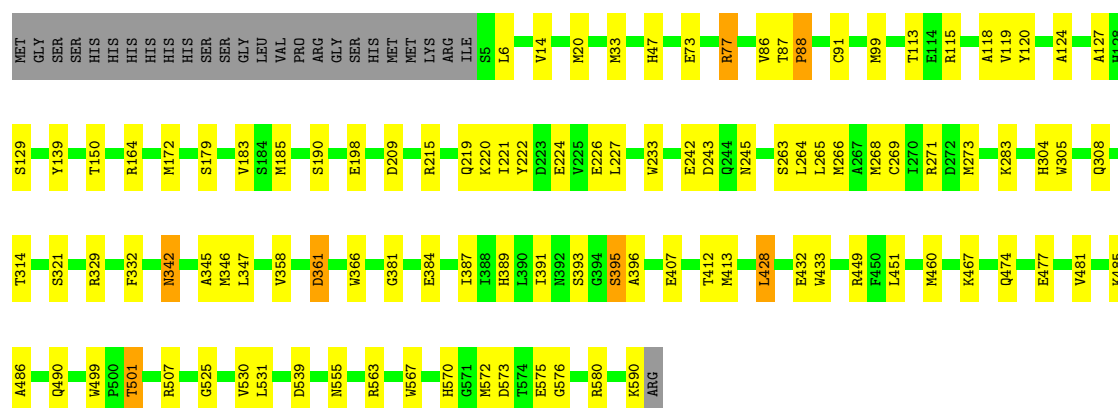
• Molecule 1: L-fucose isomerase





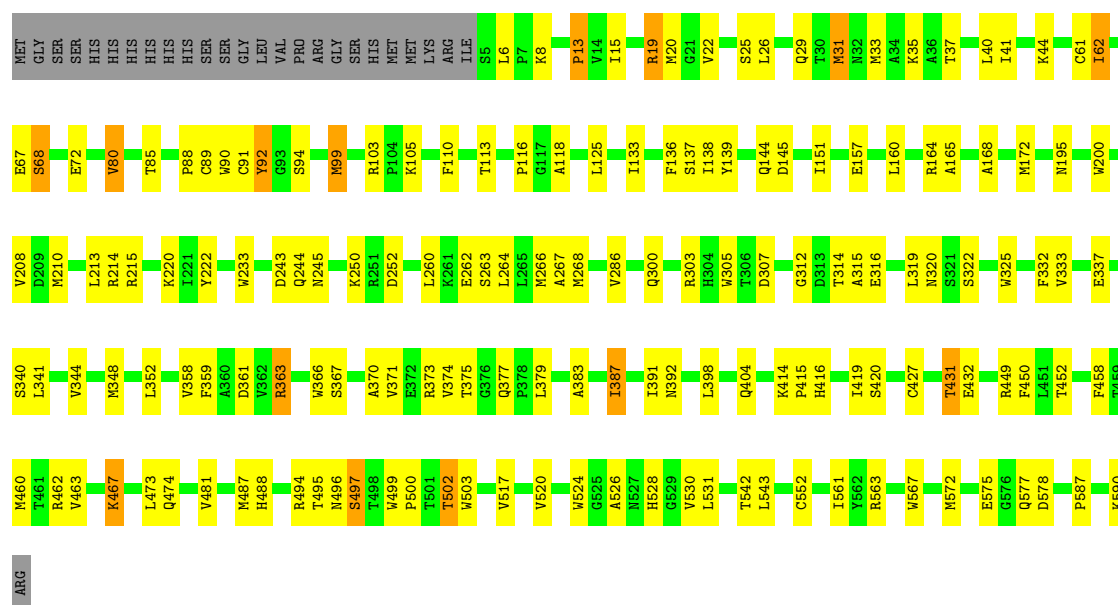
• Molecule 1: L-fucose isomerase

Chain D: 78% 16% . .



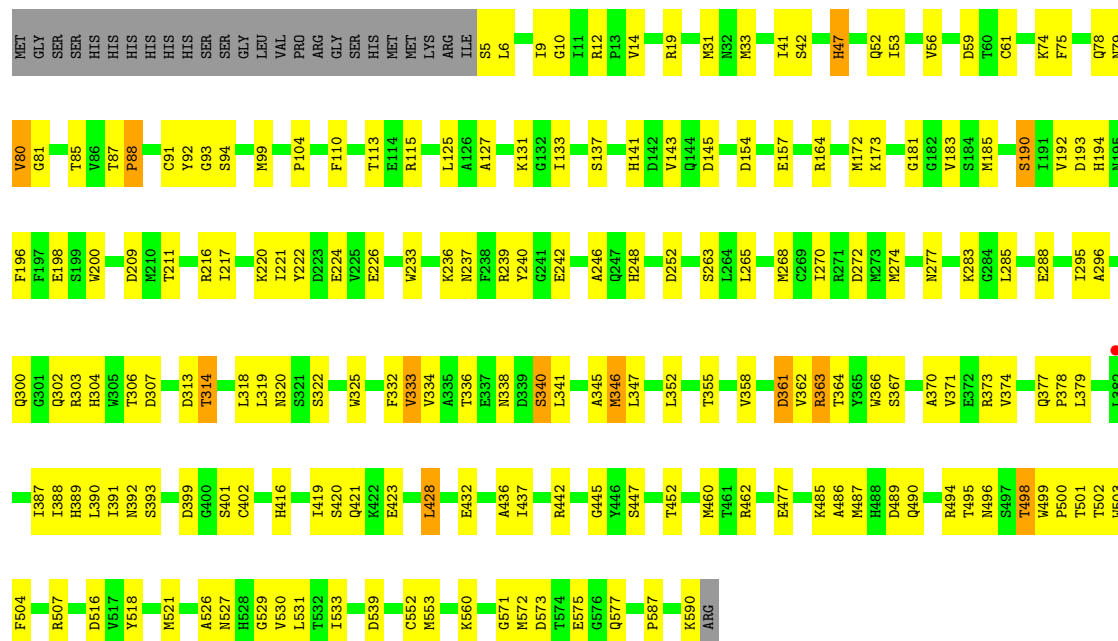
• Molecule 1: L-fucose isomerase

Chain E: 69% 24% . .



● Molecule 1: L-fucose isomerase

Chain F:  65% 29% . .



4 Data and refinement statistics

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 30.00 – 2.96	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-2.96) 93.6 (30.00-2.96)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.82%)	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 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.75	0/4609	0.90	1/6247 (0.0%)
1	B	0.70	0/4609	0.89	1/6247 (0.0%)
1	C	0.70	0/4609	0.89	2/6247 (0.0%)
1	D	0.74	0/4609	0.88	0/6247
1	E	0.69	0/4609	0.91	5/6247 (0.1%)
1	F	0.68	0/4609	0.89	1/6247 (0.0%)
All	All	0.71	0/27654	0.89	10/37482 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	MET	N-CA-C	6.65	118.53	111.28
1	F	87	THR	N-CA-C	6.19	113.79	108.22
1	C	358	VAL	N-CA-C	6.07	116.44	107.15
1	E	363	ARG	N-CA-C	5.82	118.50	111.40
1	C	87	THR	N-CA-C	5.63	115.37	108.11
1	E	19	ARG	N-CA-C	5.21	113.06	108.78
1	E	151	ILE	CA-C-N	5.21	125.19	120.03
1	E	151	ILE	C-N-CA	5.21	125.19	120.03
1	E	33	MET	N-CA-C	-5.16	105.55	111.07
1	A	328	VAL	N-CA-C	5.10	115.68	109.30

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	81	2
1	B	4508	0	4372	74	0
1	C	4508	0	4372	124	1
1	D	4508	0	4372	72	1
1	E	4508	0	4372	125	0
1	F	4508	0	4372	142	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	548	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 (548) 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:33:MET:HE2	1:D:86:VAL:HB	1.62	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:185:MET:HE3	1:C:302:GLN:HB2	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:495:THR:C	1:C:496:ASN:HD22	2.04	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
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:F:460:MET:HE2	1:F:529:GLY:HA3	1.81	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:590:LYS:C	3:F:701:HOH:O	2.42	0.62
1:F:157:GLU:OE2	1:F:560:LYS:NZ	2.32	0.62
1:F:272:ASP:CG	1:F:277:ASN:HB2	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:379:LEU:HD23	1:F:487:MET:HE1	1.84	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:C:320:ASN:OD1	1:C:346:MET:HE1	2.01	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: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: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
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:E:374:VAL:HG13	1:E:375:THR:HG23	1.86	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:A:346:MET:HE2	1:A:359:PHE:HD2	1.70	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:224:GLU:HG3	1:D:283:LYS:HZ2	1.69	0.57
1:A:221:ILE:HG23	1:A:285:LEU:HD13	1.87	0.56
1:E:590:LYS:C	3:E:702:HOH:O	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:235:ASP:CG	1:C:257:ARG:HH12	2.14	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:33:MET:HE1	1:A:87:THR:C	2.32	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
1:D:33:MET:CE	1:D:86:VAL:HB	2.35	0.55
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:F:33:MET:HE1	1:F:110:PHE:HB2	1.89	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:F:334:VAL:O	1:F:346:MET:HE1	2.06	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:B:145:ASP:CG	1:E:373:ARG:HH22	2.14	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:E:145:ASP:CG	1:F:494:ARG:NH2	2.66	0.54
1:C:260:LEU:HD23	1:C:260:LEU:O	2.08	0.54
1:C:396:ALA:O	1:C:397:ALA:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:VAL:HB	1:C:299:PHE:HA	1.89	0.53
1:C:204:LYS:HD3	1:E:99:MET:HE3	1.90	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:B:131:LYS:O	1:D:590:LYS:NZ	2.39	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:266:MET:HE1	1:E:312:GLY:HA2	1.91	0.52
1:E:415:PRO:O	1:E:419:ILE:HG13	2.10	0.52
1:F:379:LEU:CD2	1:F:487:MET:HE1	2.40	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
1:E:61:CYS:O	1:E:67:GLU:CD	2.53	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:49:CYS:C	1:C:416:HIS:HE2	2.19	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:D:266:MET:HE3	1:D:305:TRP:CZ2	2.46	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: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
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:357:GLN:OE1	1:B:532:THR:OG1	2.25	0.49
1:D:507:ARG:NH1	1:D:555:ASN:O	2.44	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: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:C:383:ALA:O	1:C:384:GLU:C	2.55	0.48
1:B:321:SER:O	1:B:329:ARG:NH1	2.46	0.48
1:D:224:GLU:HG3	1:D:283:LYS:HZ1	1.79	0.48
1:C:185:MET:HE3	1:C:302:GLN:CB	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:ASP:HB2	1:D:391:ILE:O	2.13	0.48
1:E:13:PRO:HG2	1:E:31:MET:HE2	1.94	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:B:292:TYR:O	1:B:293:ASN:C	2.57	0.47
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
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:14:VAL:HG23	1:A:87:THR:HB	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:296:ALA:HA	1:F:333:VAL:HG13	1.95	0.47
1:F:362:VAL:HG22	1:F:521:MET:HE1	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:B:158:LYS:O	1:B:159:LEU:C	2.56	0.46
1:C:233:TRP:CZ2	1:C:428:LEU:HD11	2.50	0.46
1:C:488:HIS:ND1	1:C:488:HIS:C	2.74	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
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: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: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:A:483:LEU:HB3	1:A:487:MET:HE2	1.97	0.46
1:D:226:GLU:HB3	1:D:268:MET:HE1	1.97	0.46
1:E:145:ASP:CG	1:F:373:ARG:NH2	2.74	0.46
1:F:6:LEU:HD13	1:F:47:HIS:CD2	2.51	0.46
1:A:588:LEU:HB3	1:A:589:TYR:CD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:GLN:HA	1:C:338:ASN:HB2	1.98	0.45
1:F:240:TYR:C	1:F:432:GLU:HG2	2.41	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: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:A:442:ARG:HG2	1:D:20:MET:HE1	1.98	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:90:TRP:HE1	1:F:185:MET:HE3	1.82	0.45
1:E:92:TYR:OH	1:F:303:ARG:HD2	2.17	0.45
1:F:172:MET:O	1:F:173:LYS:C	2.59	0.45
1:A:56:VAL:HG12	1:A:75:PHE:CE1	2.52	0.44
1:E:90:TRP:NE1	1:F:185:MET:HE3	2.32	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: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:158:LYS:NZ	3:A:701:HOH:O	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:22:VAL:O	1:A:25:SER:OG	2.34	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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:99:MET:HE1	1:F:198:GLU:OE2	2.19	0.42
1:B:222:TYR:CD1	1:B:265:LEU:CD2	3.01	0.42
1:B:311:ASN:OD1	1:B:311:ASN:C	2.62	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:C:185:MET:CE	1:C:302:GLN:CD	2.92	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:99:MET:HE1	1:B:131:LYS:CD	2.50	0.42
1:B:329:ARG:NH1	1:B:331:PRO:HA	2.33	0.42
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:C:483:LEU:HD13	1:C:487:MET:HE2	2.02	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:E:487:MET:HE2	1:E:487:MET:HB3	1.95	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:210:MET:HE3	1:F:211:THR:HG21	2.02	0.42
1:C:285:LEU:HD22	1:C:288:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:313:ASP:OD2	1:A:447:SER:OG	2.32	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:B:488:HIS:CD2	1:B:488:HIS:C	2.98	0.42
1:B:521:MET:HE2	1:B:521:MET:HB3	1.82	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:D:412:THR:OG1	1:D:413:MET:N	2.52	0.41
1:F:242:GLU:CD	1:F:242:GLU:H	2.28	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:D:183:VAL:HA	1:D:190:SER:CB	2.51	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:99:MET:HE1	1:B:131:LYS:HD3	2.02	0.41
1:C:19:ARG:O	1:C:20:MET:HB2	2.20	0.41
1:D:304:HIS:NE2	1:E:208:VAL:HG13	2.36	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:172:MET:O	1:C:173:LYS:C	2.63	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:B:26:LEU:O	1:B:27:GLU:C	2.63	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:F:31:MET:HE2	1:F:61:CYS:SG	2.61	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:359:PHE:C	1:E:392:ASN:ND2	2.79	0.40
1:E:427:CYS:O	1:E:431:THR:HG23	2.20	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:442:ARG:CZ	1:D:20:MET:HE3	2.51	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 [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	584/612 (95%)	556 (95%)	24 (4%)	4 (1%)	18	40
1	B	584/612 (95%)	553 (95%)	29 (5%)	2 (0%)	36	59
1	C	584/612 (95%)	540 (92%)	38 (6%)	6 (1%)	12	32
1	D	584/612 (95%)	562 (96%)	21 (4%)	1 (0%)	43	66
1	E	584/612 (95%)	552 (94%)	26 (4%)	6 (1%)	12	32
1	F	584/612 (95%)	550 (94%)	27 (5%)	7 (1%)	10	28
All	All	3504/3672 (95%)	3313 (94%)	165 (5%)	26 (1%)	18	40

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%)	455 (98%)	11 (2%)	43	67
1	B	466/489 (95%)	451 (97%)	15 (3%)	34	59
1	C	466/489 (95%)	454 (97%)	12 (3%)	40	65
1	D	466/489 (95%)	454 (97%)	12 (3%)	40	65
1	E	466/489 (95%)	441 (95%)	25 (5%)	20	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	466/489 (95%)	453 (97%)	13 (3%)	38	62
All	All	2796/2934 (95%)	2708 (97%)	88 (3%)	35	59

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	43	GLU
1	A	60	THR
1	A	91	CYS
1	A	94	SER
1	A	137	SER
1	A	336	THR
1	A	428	LEU
1	A	496	ASN
1	A	498	THR
1	A	521	MET
1	B	14	VAL
1	B	49	CYS
1	B	113	THR
1	B	251	ARG
1	B	278	GLU
1	B	336	THR
1	B	362	VAL
1	B	374	VAL
1	B	391	ILE
1	B	418	GLU
1	B	428	LEU
1	B	447	SER
1	B	497	SER
1	B	521	MET
1	B	574	THR
1	C	6	LEU
1	C	73	GLU
1	C	80	VAL
1	C	172	MET
1	C	286	VAL
1	C	342	ASN
1	C	374	VAL
1	C	384	GLU
1	C	387	ILE
1	C	420	SER

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Mol	Chain	Res	Type
1	C	428	LEU
1	C	487	MET
1	D	77	ARG
1	D	129	SER
1	D	150	THR
1	D	179	SER
1	D	263	SER
1	D	342	ASN
1	D	361	ASP
1	D	393	SER
1	D	395	SER
1	D	407	GLU
1	D	428	LEU
1	D	501	THR
1	E	29	GLN
1	E	31	MET
1	E	62	ILE
1	E	68	SER
1	E	80	VAL
1	E	85	THR
1	E	91	CYS
1	E	92	TYR
1	E	94	SER
1	E	99	MET
1	E	138	ILE
1	E	157	GLU
1	E	214	ARG
1	E	252	ASP
1	E	262	GLU
1	E	322	SER
1	E	333	VAL
1	E	367	SER
1	E	377	GLN
1	E	387	ILE
1	E	420	SER
1	E	431	THR
1	E	467	LYS
1	E	497	SER
1	E	502	THR
1	F	52	GLN
1	F	80	VAL
1	F	94	SER

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Mol	Chain	Res	Type
1	F	190	SER
1	F	226	GLU
1	F	314	THR
1	F	333	VAL
1	F	340	SER
1	F	361	ASP
1	F	363	ARG
1	F	364	THR
1	F	428	LEU
1	F	498	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	GLN
1	A	302	GLN
1	A	385	HIS
1	B	130	GLN
1	B	244	GLN
1	B	293	ASN
1	B	385	HIS
1	B	438	HIS
1	B	474	GLN
1	C	245	ASN
1	C	338	ASN
1	C	438	HIS
1	C	464	ASN
1	C	496	ASN
1	C	577	GLN
1	D	351	GLN
1	D	464	ASN
1	E	206	GLN
1	E	244	GLN
1	E	302	GLN
1	E	357	GLN
1	E	385	HIS
1	E	404	GLN
1	F	79	ASN
1	F	144	GLN
1	F	320	ASN
1	F	357	GLN
1	F	377	GLN

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Mol	Chain	Res	Type
1	F	392	ASN
1	F	404	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	586/612 (95%)	-0.52	0	100	100	28, 52, 76, 96	0
1	B	586/612 (95%)	-0.43	0	100	100	29, 58, 85, 107	0
1	C	586/612 (95%)	-0.26	0	100	100	30, 61, 89, 111	0
1	D	586/612 (95%)	-0.62	0	100	100	27, 48, 72, 100	0
1	E	586/612 (95%)	-0.22	0	100	100	36, 67, 92, 118	0
1	F	586/612 (95%)	-0.10	1 (0%)	91	90	33, 71, 101, 127	0
All	All	3516/3672 (95%)	-0.36	1 (0%)	100	100	27, 59, 90, 127	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	382	LEU	2.6

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](#)

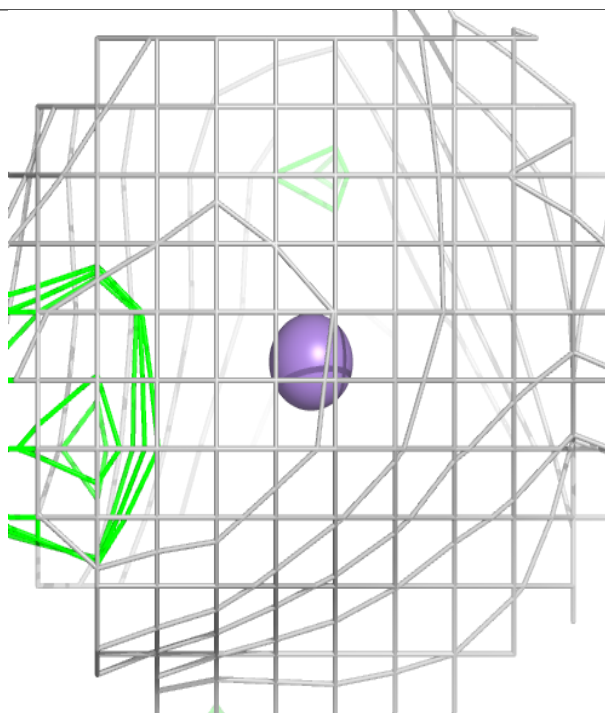
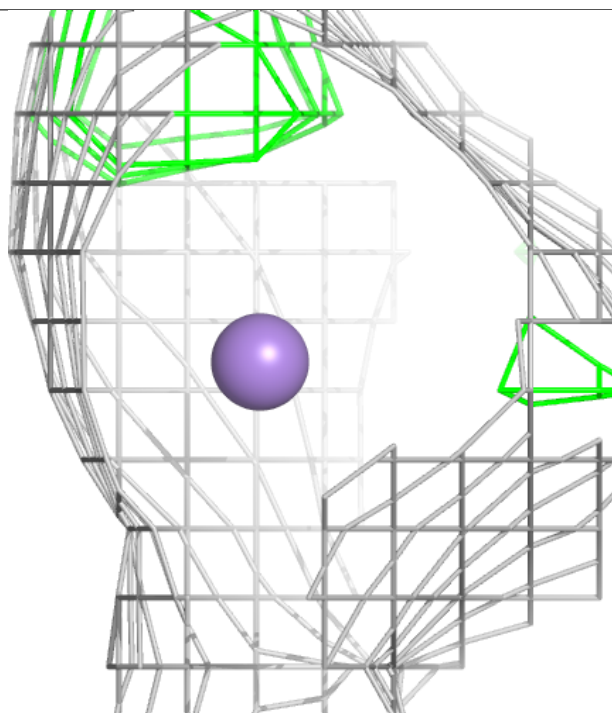
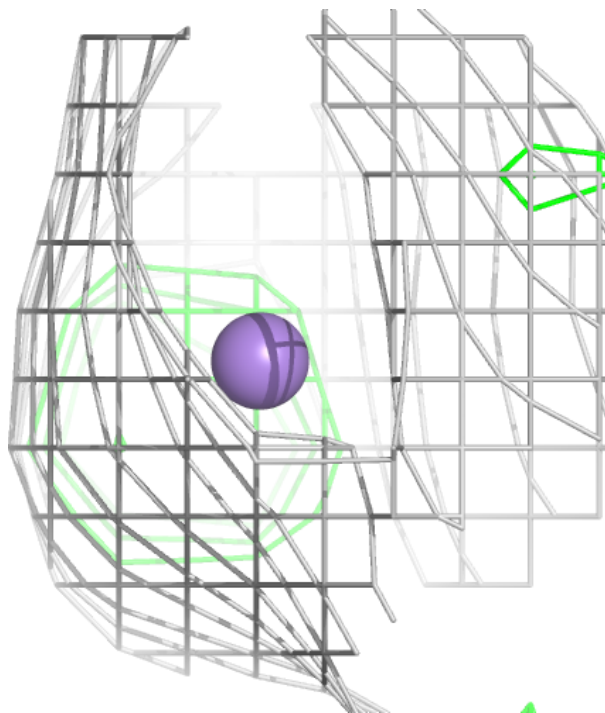
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	F	601	1/1	0.86	0.09	90,90,90,90	0
2	MN	E	601	1/1	0.93	0.05	81,81,81,81	0
2	MN	B	601	1/1	0.93	0.07	64,64,64,64	0
2	MN	D	601	1/1	0.95	0.05	73,73,73,73	0
2	MN	C	601	1/1	0.97	0.05	74,74,74,74	0
2	MN	A	601	1/1	0.97	0.04	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.

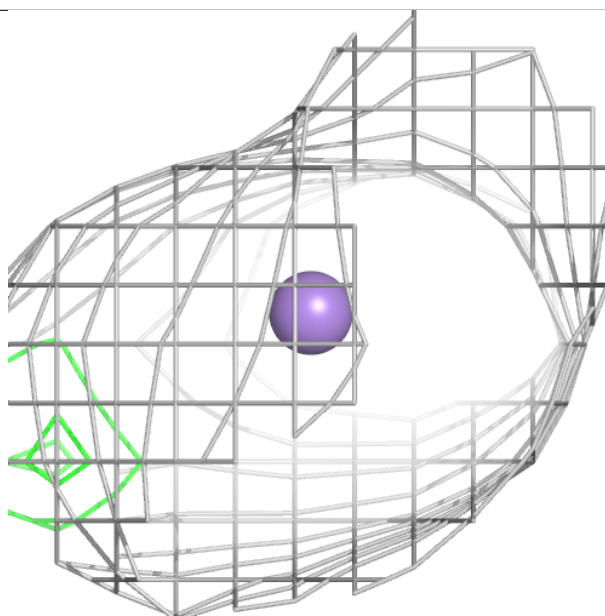
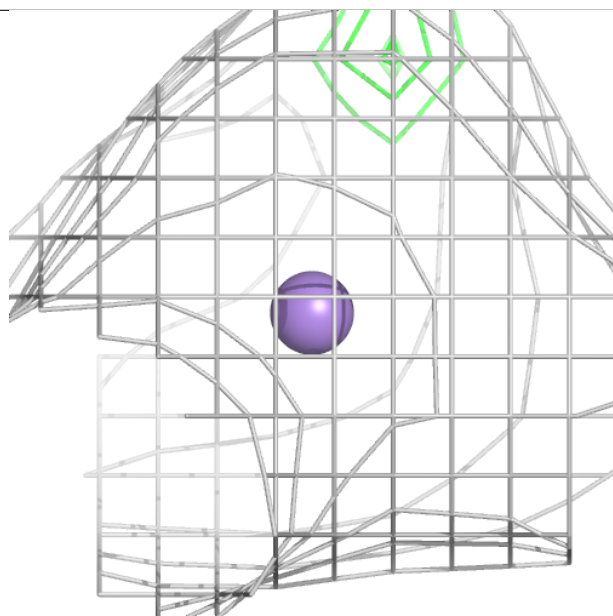
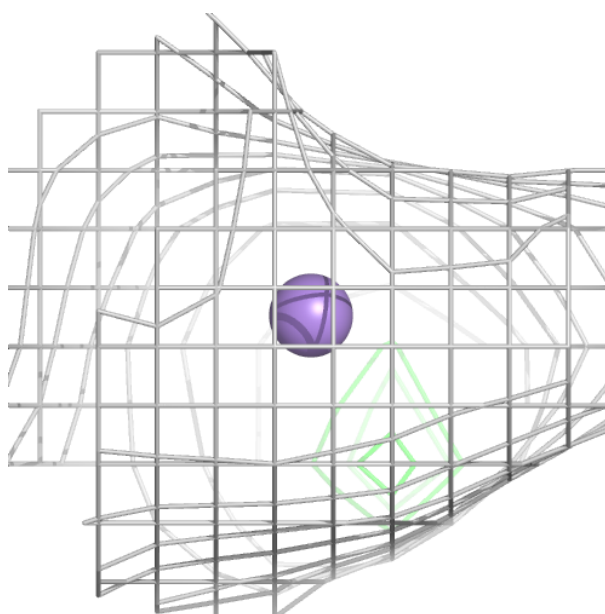
Electron density around MN F 601:

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



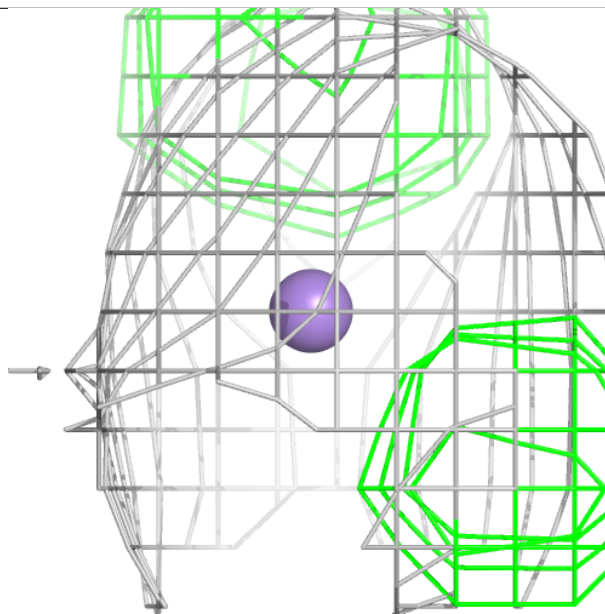
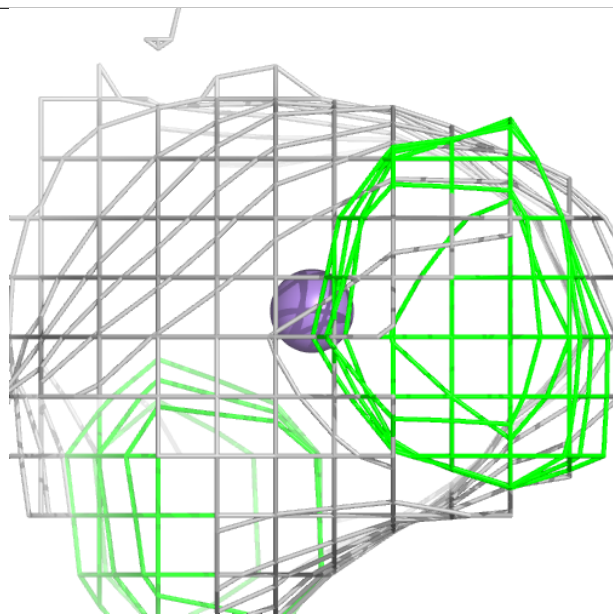
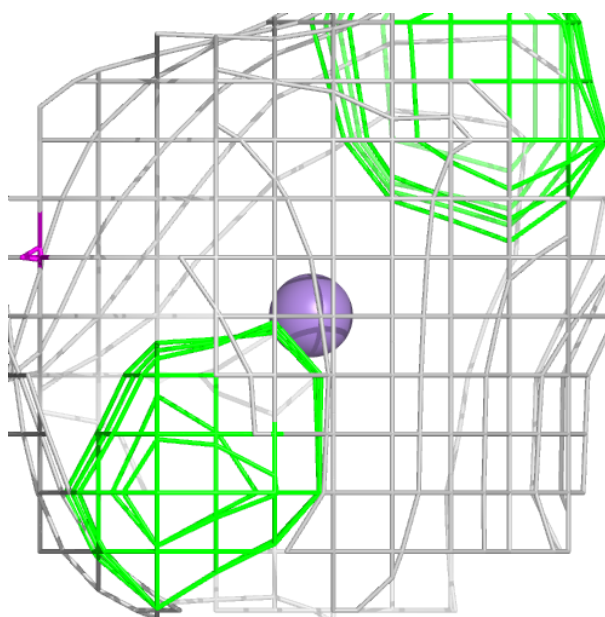
Electron density around MN E 601:

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



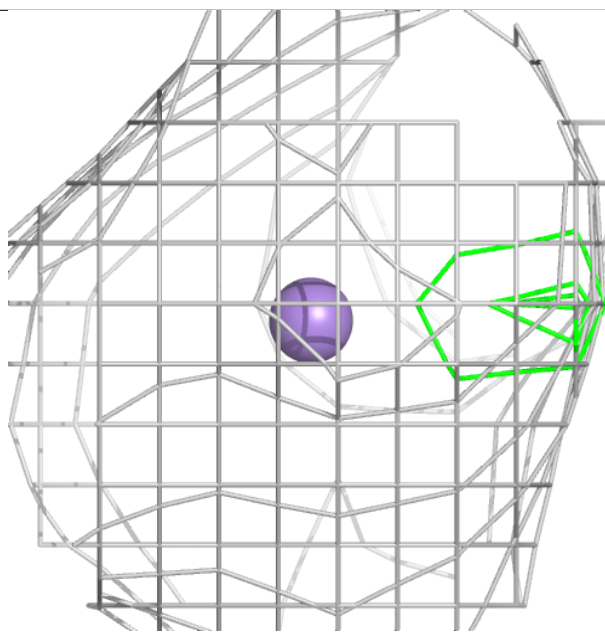
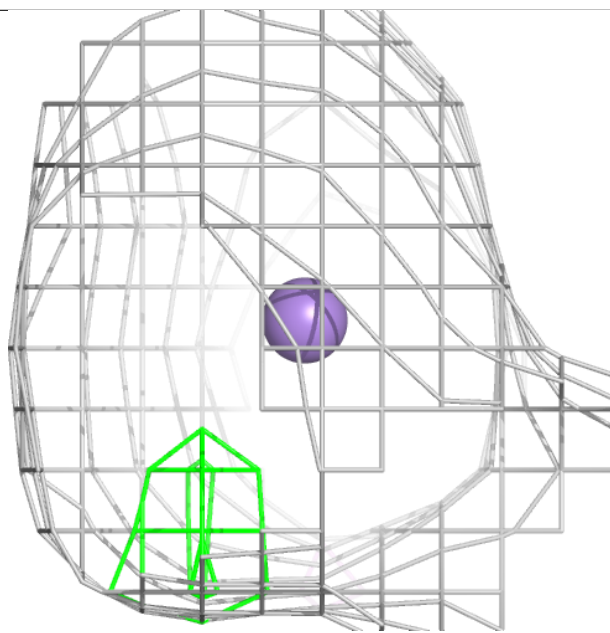
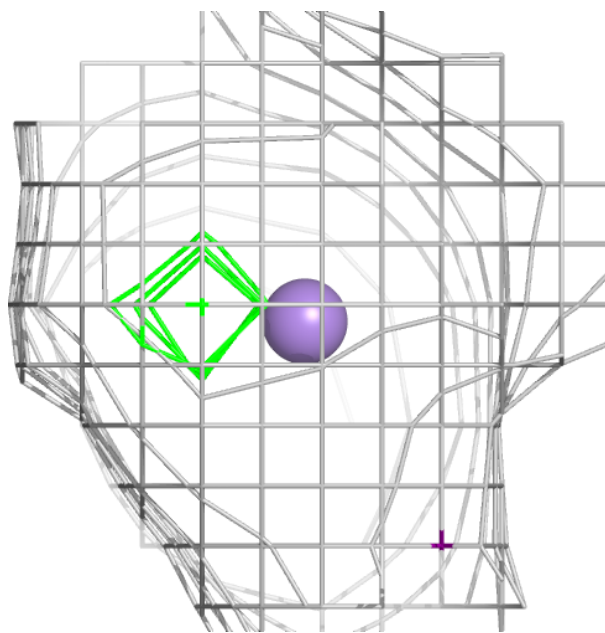
Electron density around MN B 601:

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



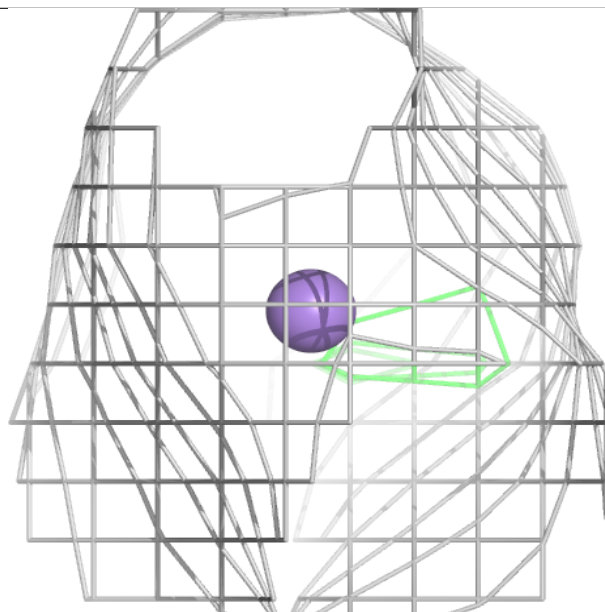
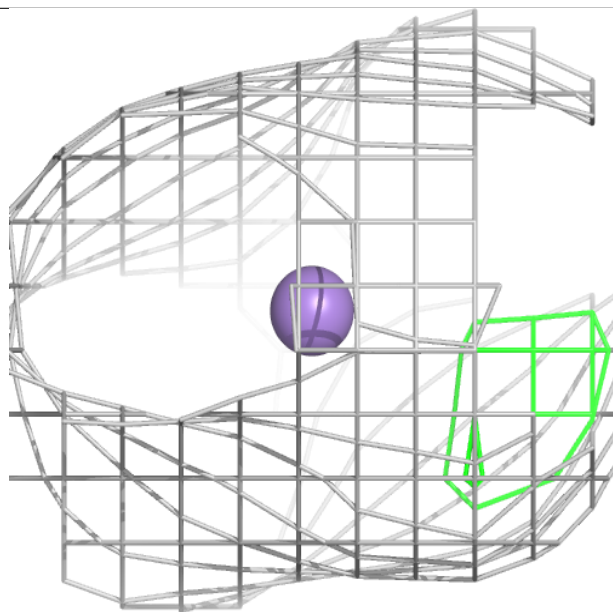
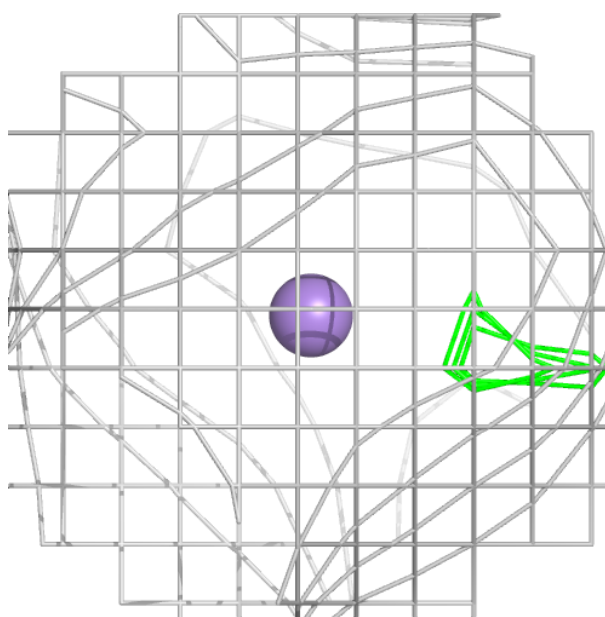
Electron density around MN D 601:

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



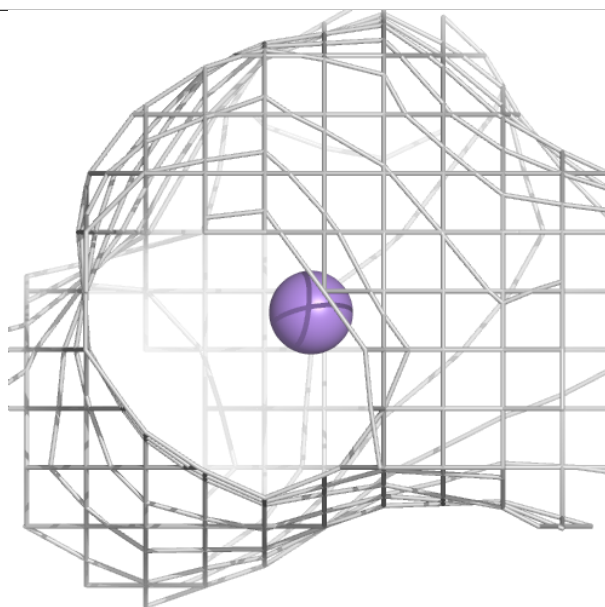
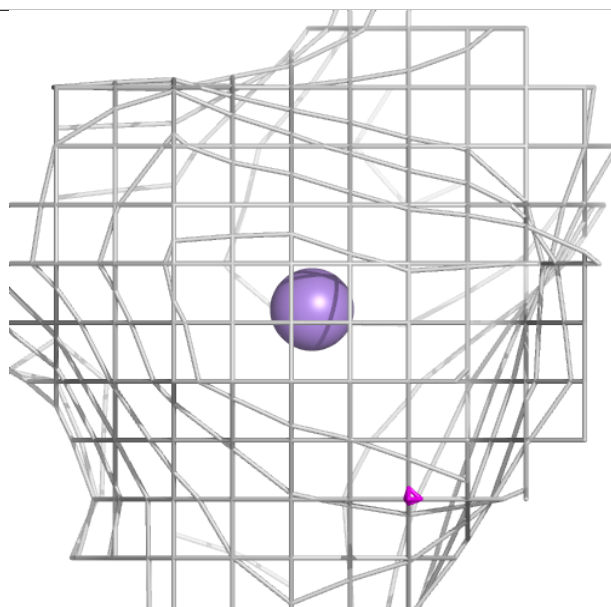
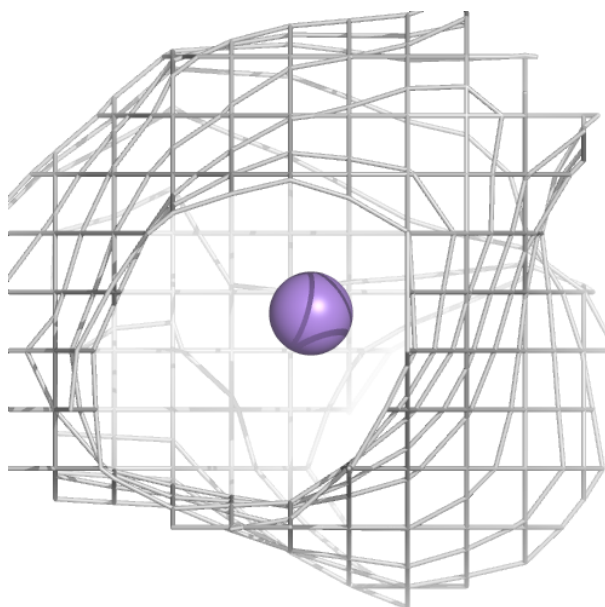
Electron density around MN C 601:

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



Electron density around MN A 601:

$2mF_o-DF_c$ (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.