



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2025 – 05:17 PM JST

PDB ID : 9WF6 / pdb_00009wf6
Title : Crystal Structure of Escherichia coli GroEL with Magnesium Ions and a Phosphorylated Serine Residue-3.0 Å
Authors : Guo, Y.; Zhang, L.; Zheng, H.; Li, J.; Han, Q.
Deposited on : 2025-08-21
Resolution : 2.99 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:

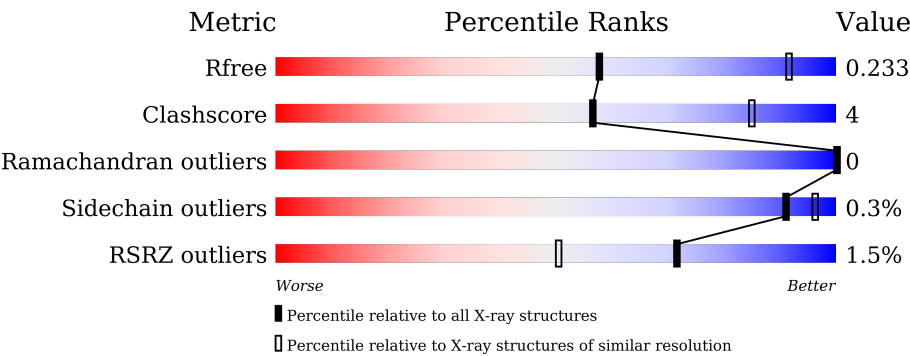
MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.99 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.






















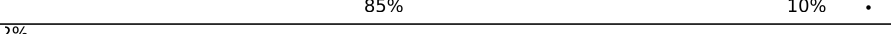


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	548	<div><div>3%</div><div><div></div><div>85%</div><div>10%</div><div>.</div></div></div>
1	B	548	<div><div>%</div><div><div></div><div>89%</div><div>7%</div><div>.</div></div></div>
1	C	548	<div><div>2%</div><div><div></div><div>87%</div><div>9%</div><div>.</div></div></div>
1	F	548	<div><div>3%</div><div><div></div><div>86%</div><div>9%</div><div>.</div></div></div>
1	G	548	<div><div>3%</div><div><div></div><div>85%</div><div>10%</div><div>.</div></div></div>
1	H	548	<div><div></div><div><div></div><div>88%</div><div>8%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	I	548	 90% 5% .
1	J	548	 89% 6% .
1	M	548	 87% 9% .
1	N	548	 89% 7% .
1	P	548	 89% 7% .
1	Q	548	 85% 11% .
1	T	548	 90% 6% .
1	U	548	 88% 8% .
1	Y	548	 85% 11% .
1	a	548	 84% 11% .
1	b	548	 87% 9% .
2	D	548	 86% 10% .
2	E	548	 88% 7% .
2	K	548	 83% 13% .
2	L	548	 85% 11% .
2	O	548	 87% 8% .
2	R	548	 86% 9% .
2	V	548	 85% 11% .
2	W	548	 85% 10% .
2	X	548	 87% 8% .
2	Z	548	 84% 11% .
2	c	548	 89% 7% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 108950 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 Chaperonin GroEL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	B	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	C	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	F	524	Total	C	N	O	P	S	0	0	0
			3859	2397	665	776	1	20			
1	G	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	H	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	I	524	Total	C	N	O	P	S	0	0	0
			3859	2397	665	776	1	20			
1	J	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	M	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	N	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	P	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	Q	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	T	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	U	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	Y	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			
1	a	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			

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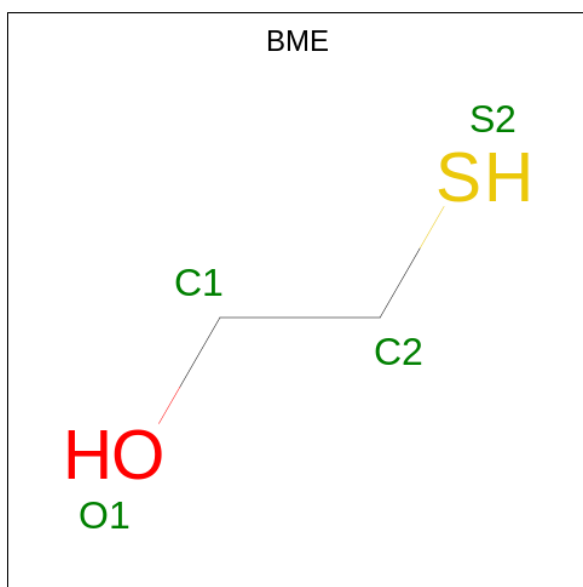
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	b	525	Total	C	N	O	P	S	0	0	0
			3868	2403	667	777	1	20			

- Molecule 2 is a protein called Chaperonin GroEL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	E	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	K	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	L	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	O	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	R	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	V	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	W	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	X	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	Z	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				
2	c	525	Total	C	N	O	S		0	0	0
			3864	2403	667	774	20				

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		
3	E	1	Total	C	O	S	0	0
			4	2	1	1		
3	E	1	Total	C	O	S	0	0
			4	2	1	1		
3	E	1	Total	C	O	S	0	0
			4	2	1	1		
3	F	1	Total	C	O	S	0	0
			4	2	1	1		
3	G	1	Total	C	O	S	0	0
			4	2	1	1		
3	G	1	Total	C	O	S	0	0
			4	2	1	1		
3	G	1	Total	C	O	S	0	0
			4	2	1	1		

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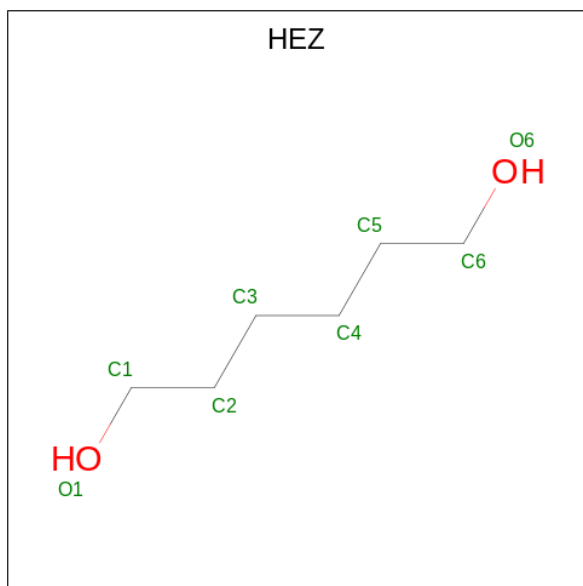
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total 4	C 2	O 1	S 1	0	0
3	H	1	Total 4	C 2	O 1	S 1	0	0
3	J	1	Total 4	C 2	O 1	S 1	0	0
3	K	1	Total 4	C 2	O 1	S 1	0	0
3	M	1	Total 4	C 2	O 1	S 1	0	0
3	N	1	Total 4	C 2	O 1	S 1	0	0
3	O	1	Total 4	C 2	O 1	S 1	0	0
3	O	1	Total 4	C 2	O 1	S 1	0	0
3	O	1	Total 4	C 2	O 1	S 1	0	0
3	P	1	Total 4	C 2	O 1	S 1	0	0
3	P	1	Total 4	C 2	O 1	S 1	0	0
3	Q	1	Total 4	C 2	O 1	S 1	0	0
3	Q	1	Total 4	C 2	O 1	S 1	0	0
3	Q	1	Total 4	C 2	O 1	S 1	0	0
3	R	1	Total 4	C 2	O 1	S 1	0	0
3	R	1	Total 4	C 2	O 1	S 1	0	0
3	T	1	Total 4	C 2	O 1	S 1	0	0
3	U	1	Total 4	C 2	O 1	S 1	0	0
3	U	1	Total 4	C 2	O 1	S 1	0	0
3	U	1	Total 4	C 2	O 1	S 1	0	0
3	V	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	X	1	Total	C	O	S	0	0
			4	2	1	1		
3	X	1	Total	C	O	S	0	0
			4	2	1	1		
3	Y	1	Total	C	O	S	0	0
			4	2	1	1		
3	Z	1	Total	C	O	S	0	0
			4	2	1	1		
3	a	1	Total	C	O	S	0	0
			4	2	1	1		
3	b	1	Total	C	O	S	0	0
			4	2	1	1		
3	c	1	Total	C	O	S	0	0
			4	2	1	1		
3	c	1	Total	C	O	S	0	0
			4	2	1	1		
3	c	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is HEXANE-1,6-DIOL (CCD ID: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	J	1	Total	C	O	0	0
			8	6	2		
4	K	1	Total	C	O	0	0
			8	6	2		
4	L	1	Total	C	O	0	0
			8	6	2		
4	M	1	Total	C	O	0	0
			8	6	2		
4	N	1	Total	C	O	0	0
			8	6	2		
4	O	1	Total	C	O	0	0
			8	6	2		
4	O	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	C	O	0	0
			8	6	2		
4	Q	1	Total	C	O	0	0
			8	6	2		
4	R	1	Total	C	O	0	0
			8	6	2		
4	R	1	Total	C	O	0	0
			8	6	2		
4	T	1	Total	C	O	0	0
			8	6	2		
4	T	1	Total	C	O	0	0
			8	6	2		
4	U	1	Total	C	O	0	0
			8	6	2		
4	V	1	Total	C	O	0	0
			8	6	2		
4	V	1	Total	C	O	0	0
			8	6	2		
4	W	1	Total	C	O	0	0
			8	6	2		
4	W	1	Total	C	O	0	0
			8	6	2		
4	X	1	Total	C	O	0	0
			8	6	2		
4	Y	1	Total	C	O	0	0
			8	6	2		
4	Z	1	Total	C	O	0	0
			8	6	2		
4	a	1	Total	C	O	0	0
			8	6	2		
4	b	1	Total	C	O	0	0
			8	6	2		
4	c	1	Total	C	O	0	0
			8	6	2		
4	c	1	Total	C	O	0	0
			8	6	2		
4	c	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0
5	H	2	Total Mg 2 2	0	0
5	M	1	Total Mg 1 1	0	0
5	N	1	Total Mg 1 1	0	0
5	T	1	Total Mg 1 1	0	0
5	U	1	Total Mg 1 1	0	0
5	V	1	Total Mg 1 1	0	0
5	b	1	Total Mg 1 1	0	0
5	c	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	B	7	Total O 7 7	0	0
6	C	3	Total O 3 3	0	0
6	D	9	Total O 9 9	0	0
6	E	6	Total O 6 6	0	0
6	F	6	Total O 6 6	0	0
6	G	5	Total O 5 5	0	0

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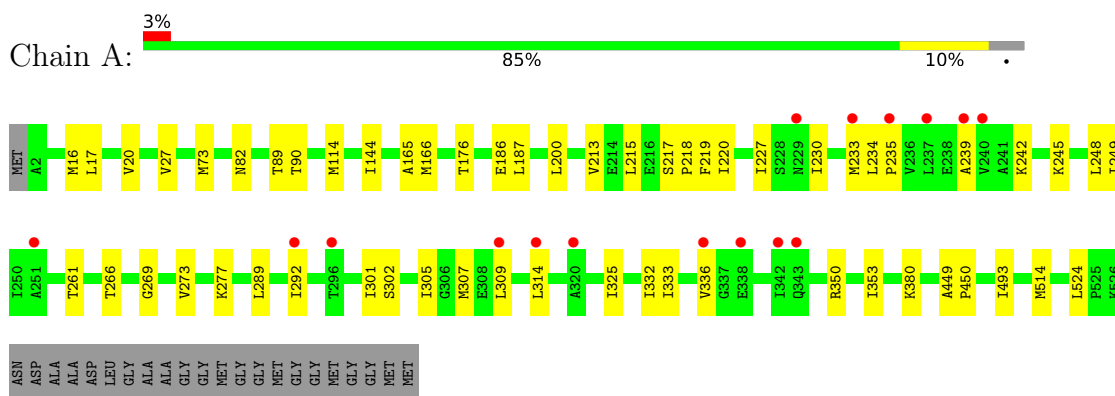
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	13	Total 13	O 13	0	0
6	I	6	Total 6	O 6	0	0
6	J	4	Total 4	O 4	0	0
6	K	5	Total 5	O 5	0	0
6	L	3	Total 3	O 3	0	0
6	M	8	Total 8	O 8	0	0
6	N	11	Total 11	O 11	0	0
6	O	9	Total 9	O 9	0	0
6	P	3	Total 3	O 3	0	0
6	Q	8	Total 8	O 8	0	0
6	R	5	Total 5	O 5	0	0
6	T	7	Total 7	O 7	0	0
6	U	9	Total 9	O 9	0	0
6	V	3	Total 3	O 3	0	0
6	W	1	Total 1	O 1	0	0
6	X	5	Total 5	O 5	0	0
6	Y	6	Total 6	O 6	0	0
6	Z	8	Total 8	O 8	0	0
6	a	9	Total 9	O 9	0	0
6	b	7	Total 7	O 7	0	0
6	c	8	Total 8	O 8	0	0

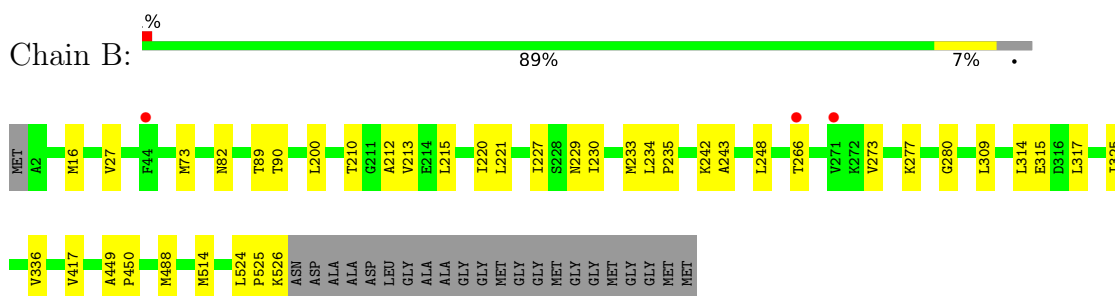
3 Residue-property plots [i](#)

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.

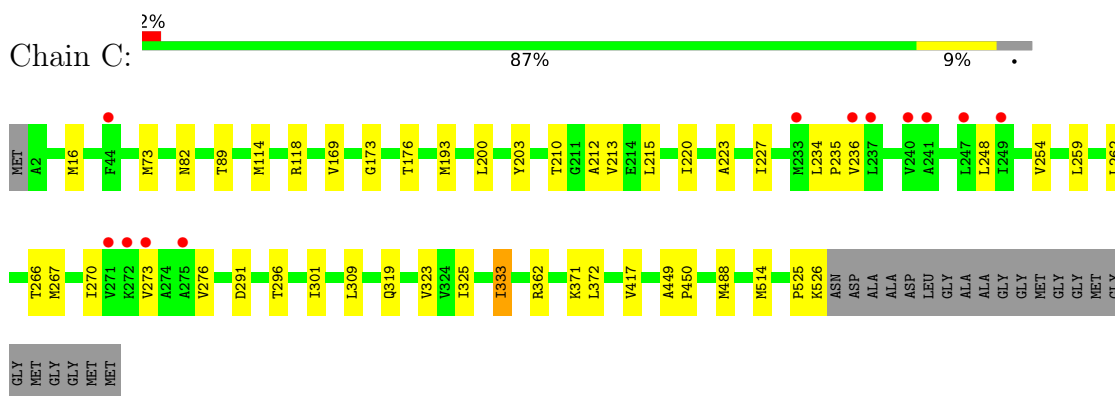
• Molecule 1: Chaperonin GroEL



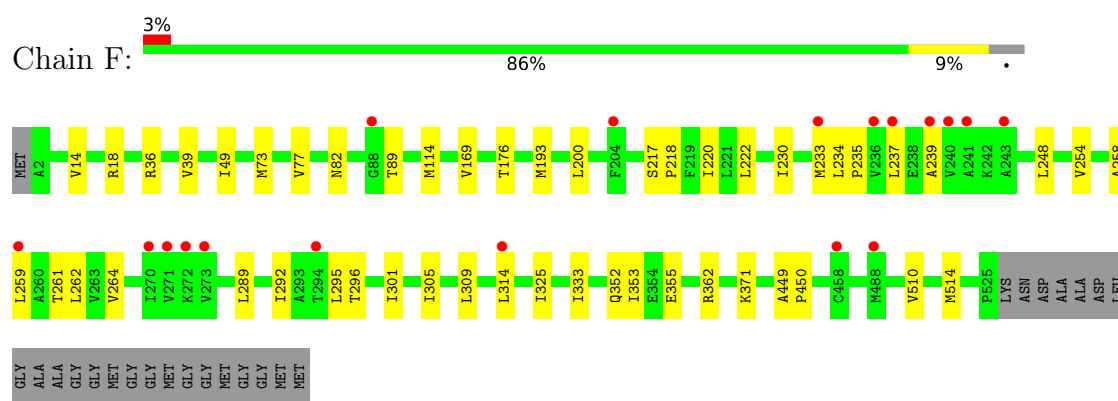
• Molecule 1: Chaperonin GroEL



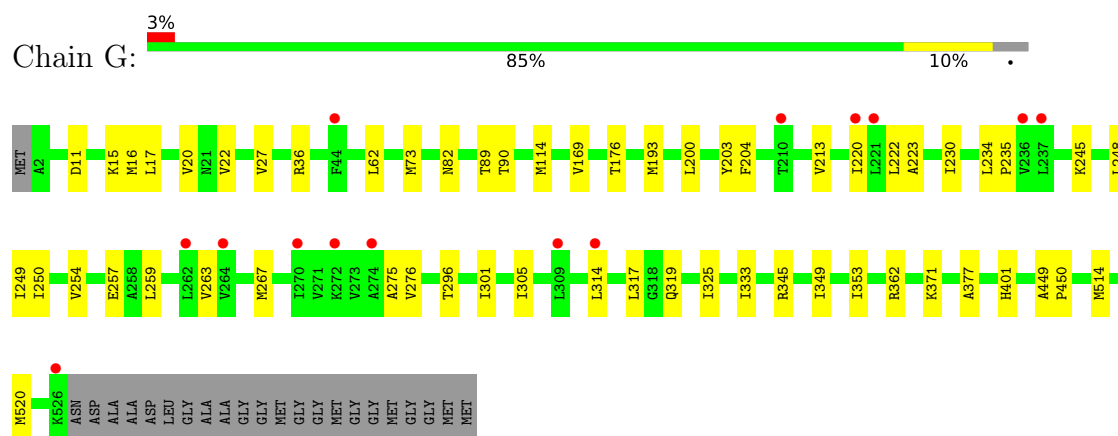
• Molecule 1: Chaperonin GroEL



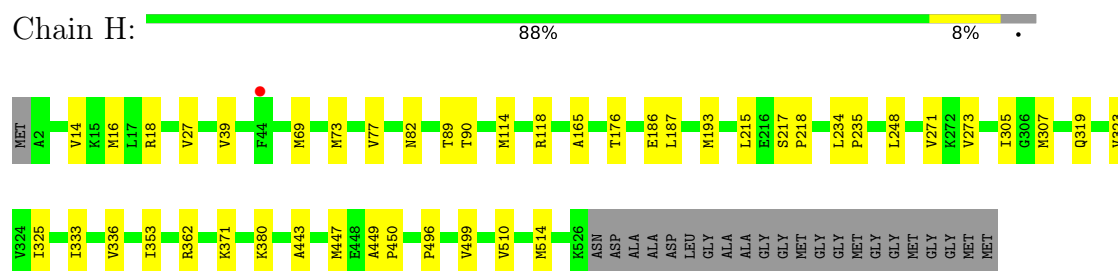
• Molecule 1: Chaperonin GroEL



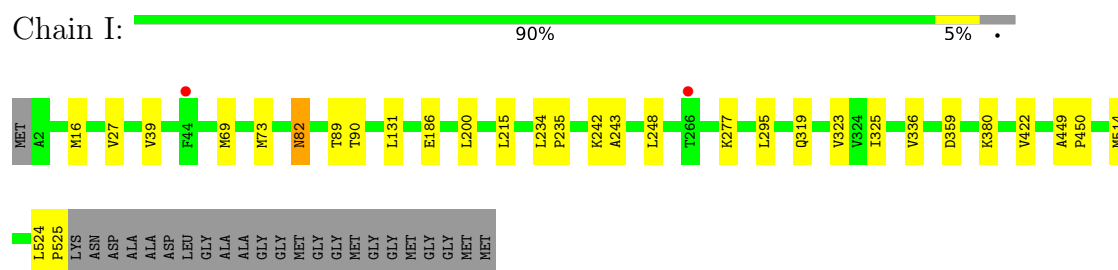
- Molecule 1: Chaperonin GroEL



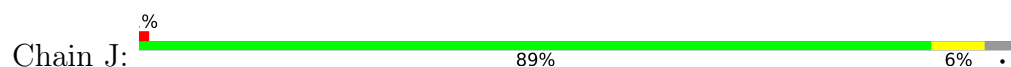
- Molecule 1: Chaperonin GroEL



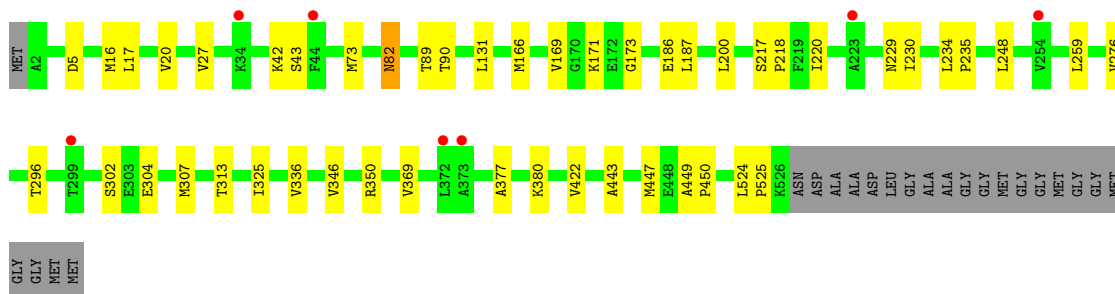
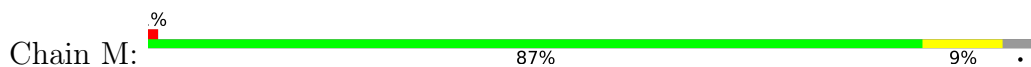
- Molecule 1: Chaperonin GroEL



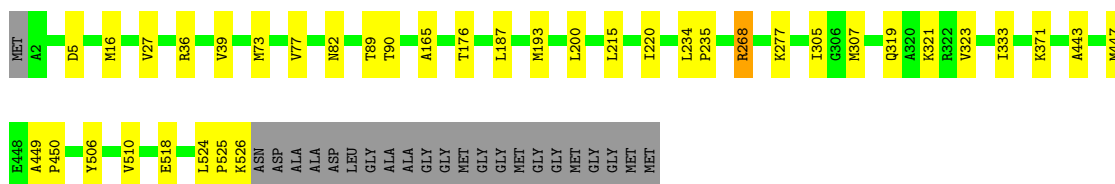
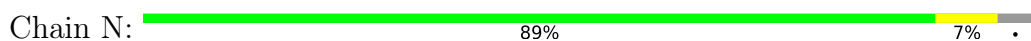
- Molecule 1: Chaperonin GroEL



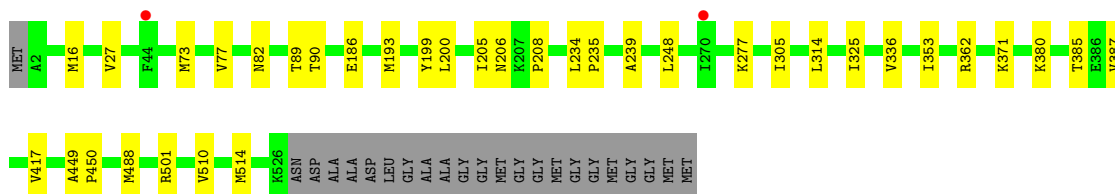
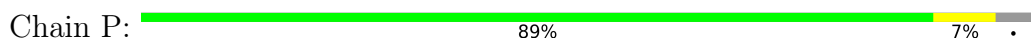
- Molecule 1: Chaperonin GroEL



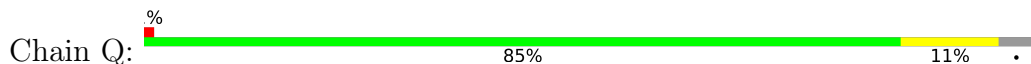
- Molecule 1: Chaperonin GroEL



- Molecule 1: Chaperonin GroEL

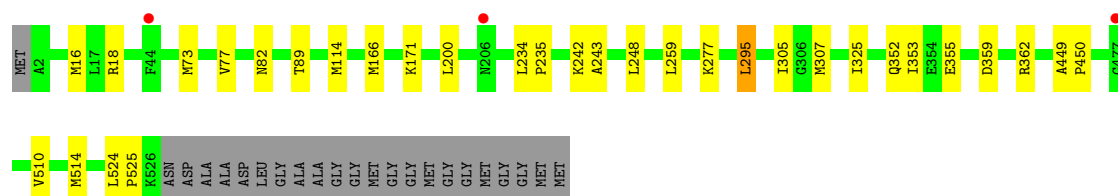
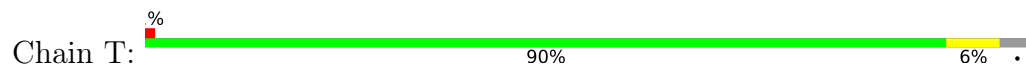


- Molecule 1: Chaperonin GroEL

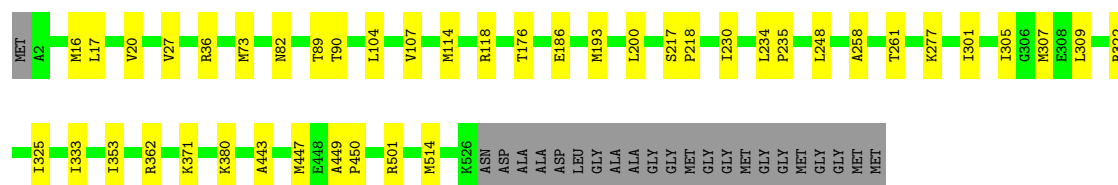
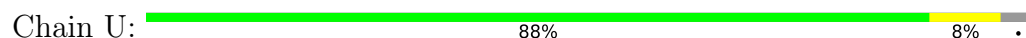




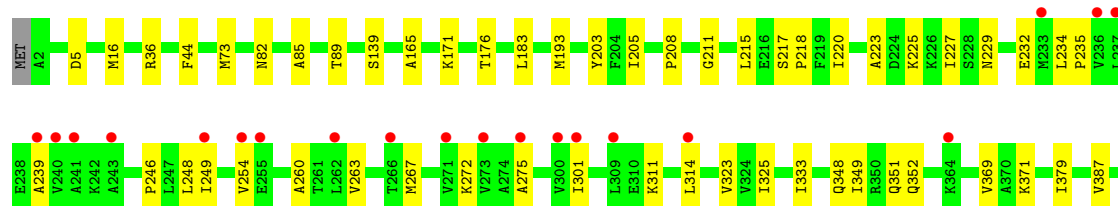
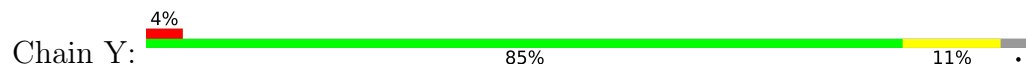
• Molecule 1: Chaperonin GroEL



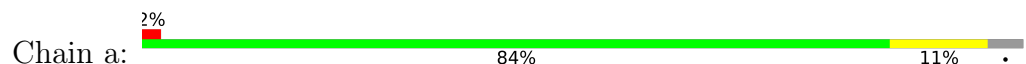
• Molecule 1: Chaperonin GroEL

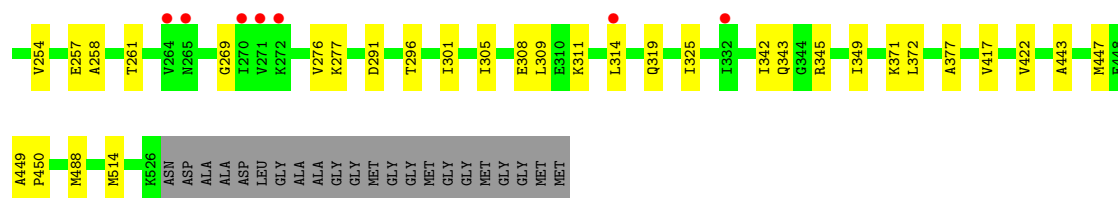


• Molecule 1: Chaperonin GroEL

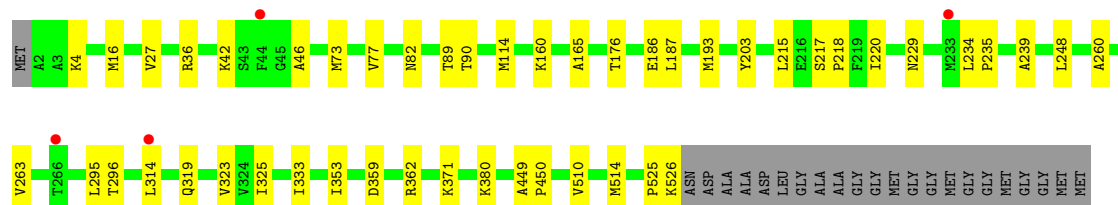
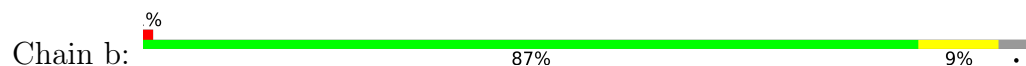


• Molecule 1: Chaperonin GroEL

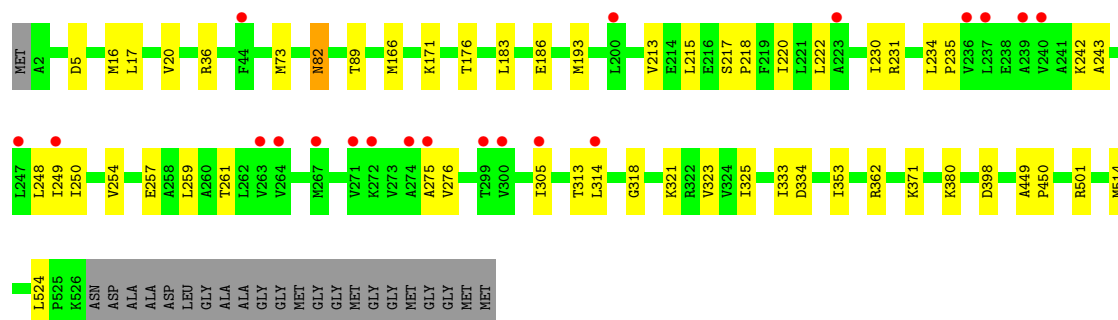
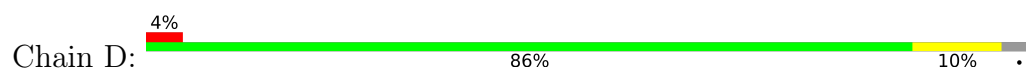




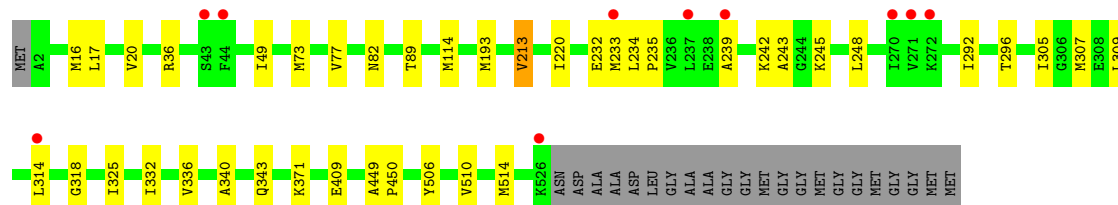
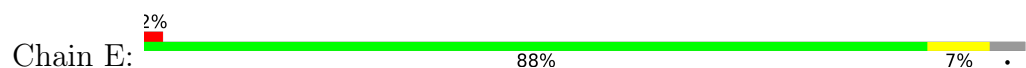
• Molecule 1: Chaperonin GroEL



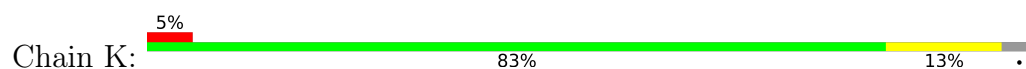
• Molecule 2: Chaperonin GroEL

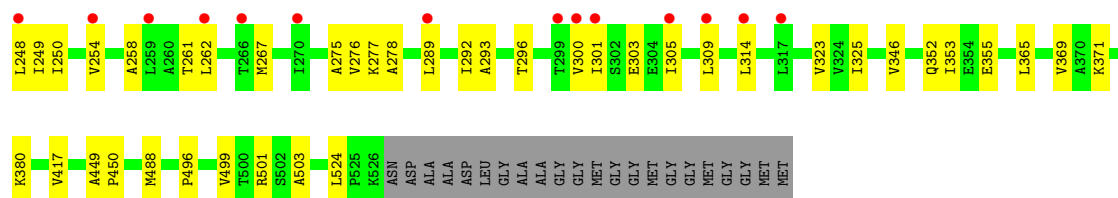


• Molecule 2: Chaperonin GroEL

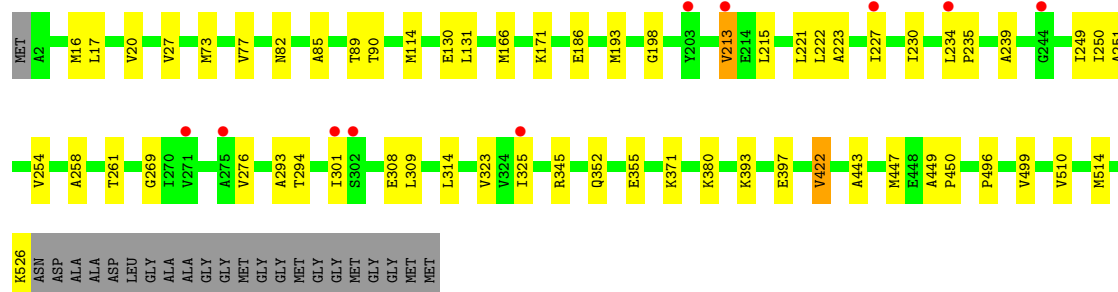
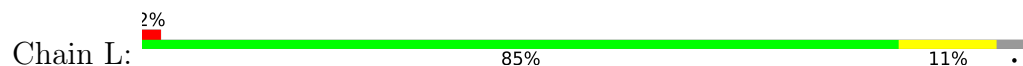


• Molecule 2: Chaperonin GroEL

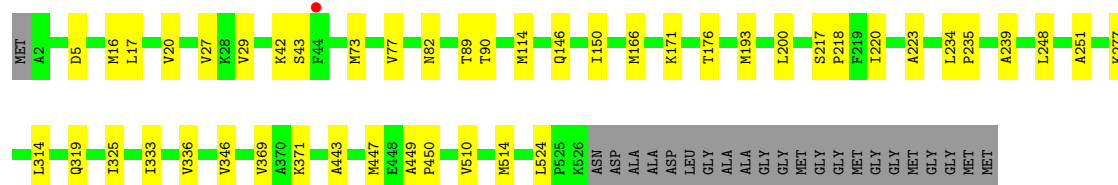
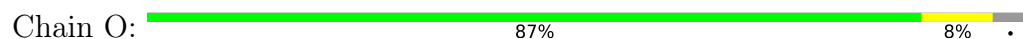




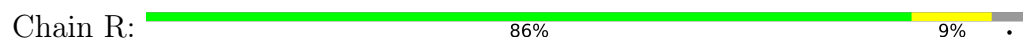
• Molecule 2: Chaperonin GroEL



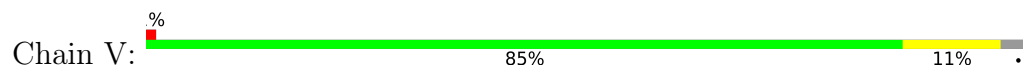
• Molecule 2: Chaperonin GroEL

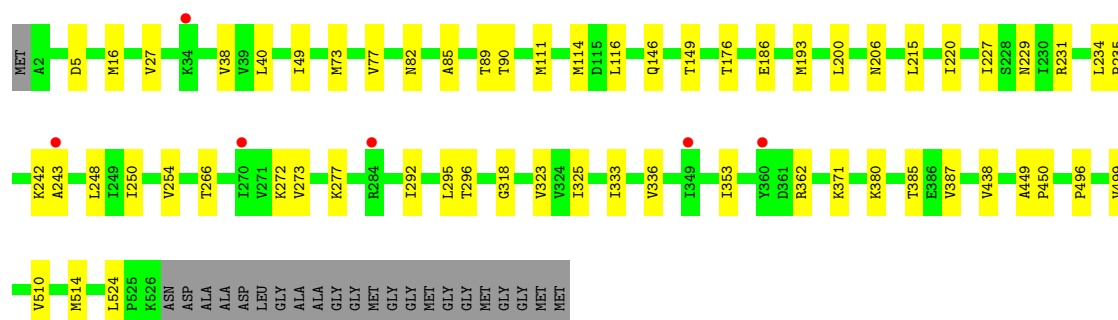


• Molecule 2: Chaperonin GroEL

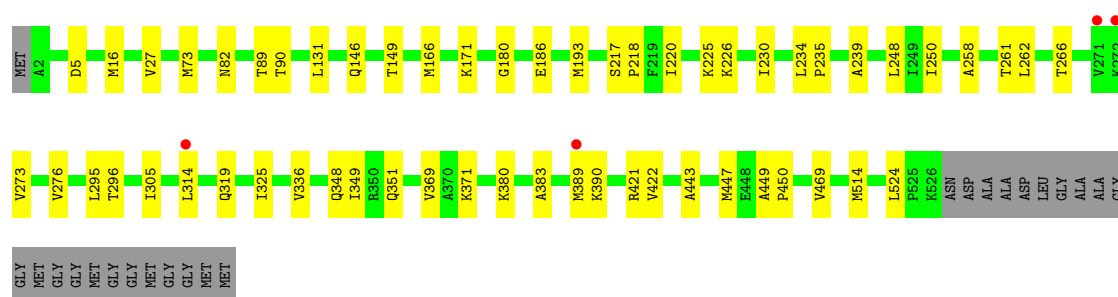
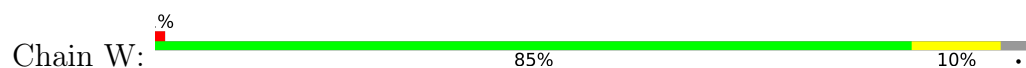


• Molecule 2: Chaperonin GroEL

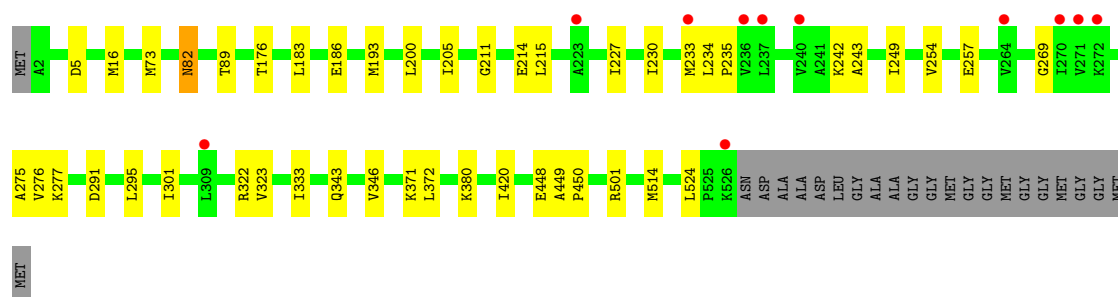
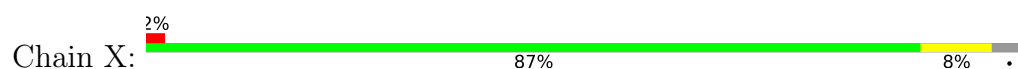




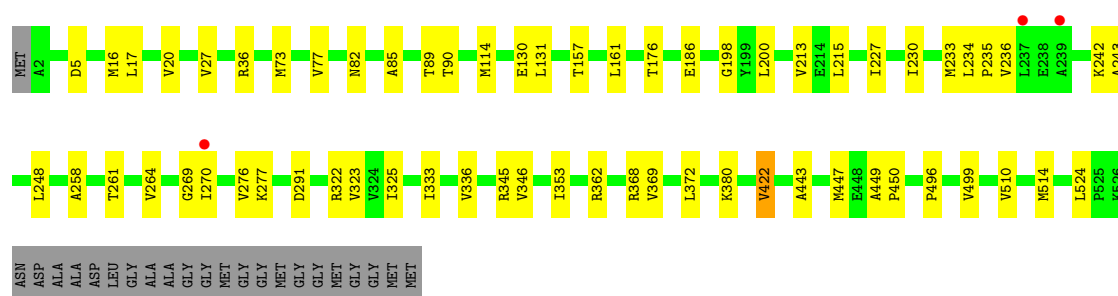
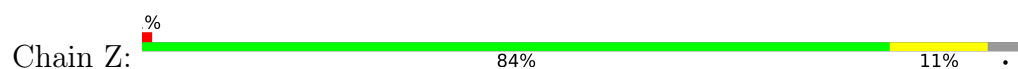
• Molecule 2: Chaperonin GroEL



• Molecule 2: Chaperonin GroEL



• Molecule 2: Chaperonin GroEL

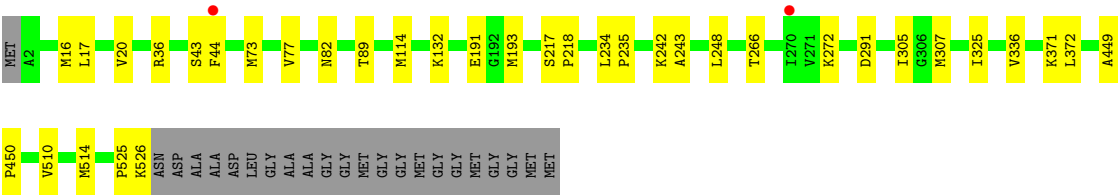


● Molecule 2: Chaperonin GroEL

Chain c:

89%

7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	285.87Å 136.26Å 287.80Å 90.00° 117.11° 90.00°	Depositor
Resolution (Å)	49.74 – 2.99 49.74 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.74-2.99) 99.0 (49.74-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.205 , 0.236 0.203 , 0.233	Depositor DCC
R_{free} test set	19672 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	108950	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: SEP, BME, MG, HEZ

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	0.51	0/3885	0.89	0/5243
1	B	0.52	0/3885	0.89	0/5243
1	C	0.51	0/3885	0.89	0/5243
1	F	0.51	0/3876	0.89	0/5232
1	G	0.51	0/3885	0.90	0/5243
1	H	0.54	0/3885	0.90	0/5243
1	I	0.55	0/3876	0.88	0/5232
1	J	0.53	0/3885	0.89	0/5243
1	M	0.52	0/3885	0.90	0/5243
1	N	0.53	0/3885	0.90	0/5243
1	P	0.52	0/3885	0.88	0/5243
1	Q	0.53	0/3885	0.88	0/5243
1	T	0.52	0/3885	0.89	0/5243
1	U	0.53	0/3885	0.88	0/5243
1	Y	0.52	0/3885	0.89	0/5243
1	a	0.52	0/3885	0.89	0/5243
1	b	0.52	0/3885	0.89	1/5243 (0.0%)
2	D	0.51	0/3892	0.89	0/5254
2	E	0.52	0/3892	0.89	0/5254
2	K	0.52	0/3892	0.90	0/5254
2	L	0.51	0/3892	0.89	0/5254
2	O	0.53	0/3892	0.89	0/5254
2	R	0.52	0/3892	0.89	0/5254
2	V	0.51	0/3892	0.89	0/5254
2	W	0.50	0/3892	0.88	0/5254
2	X	0.51	0/3892	0.89	0/5254
2	Z	0.53	0/3892	0.89	0/5254
2	c	0.52	0/3892	0.88	0/5254
All	All	0.52	0/108839	0.89	1/146903 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	359	ASP	CA-CB-CG	5.02	117.62	112.60

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	3868	0	3988	39	0
1	B	3868	0	3987	28	0
1	C	3868	0	3988	34	0
1	F	3859	0	3974	43	0
1	G	3868	0	3988	50	0
1	H	3868	0	3988	29	0
1	I	3859	0	3975	23	0
1	J	3868	0	3988	25	0
1	M	3868	0	3988	34	0
1	N	3868	0	3988	28	0
1	P	3868	0	3987	23	0
1	Q	3868	0	3987	35	0
1	T	3868	0	3988	19	0
1	U	3868	0	3988	27	0
1	Y	3868	0	3987	41	0
1	a	3868	0	3987	51	0
1	b	3868	0	3987	30	0
2	D	3864	0	3989	47	0
2	E	3864	0	3989	32	0
2	K	3864	0	3989	69	0
2	L	3864	0	3989	45	0
2	O	3864	0	3989	30	0
2	R	3864	0	3989	41	0
2	V	3864	0	3989	41	0
2	W	3864	0	3989	43	0
2	X	3864	0	3989	34	0
2	Z	3864	0	3989	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	c	3864	0	3989	26	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	C	4	0	6	0	0
3	D	12	0	18	0	0
3	E	12	0	18	1	0
3	F	4	0	6	0	0
3	G	16	0	24	1	0
3	H	4	0	6	0	0
3	J	4	0	6	0	0
3	K	4	0	6	2	0
3	M	4	0	6	1	0
3	N	4	0	6	0	0
3	O	12	0	18	1	0
3	P	8	0	12	0	0
3	Q	12	0	18	3	0
3	R	8	0	12	0	0
3	T	4	0	6	0	0
3	U	12	0	18	0	0
3	V	4	0	6	0	0
3	X	8	0	12	0	0
3	Y	4	0	6	0	0
3	Z	4	0	6	0	0
3	a	4	0	6	0	0
3	b	4	0	6	0	0
3	c	12	0	18	2	0
4	A	16	0	28	0	0
4	B	16	0	28	2	0
4	C	8	0	14	0	0
4	D	16	0	28	1	0
4	E	24	0	42	1	0
4	F	16	0	28	0	0
4	G	8	0	14	0	0
4	H	8	0	14	0	0
4	I	16	0	28	0	0
4	J	8	0	14	0	0
4	K	8	0	14	1	0
4	L	8	0	14	0	0
4	M	8	0	14	0	0
4	N	8	0	14	1	0
4	O	16	0	28	0	0
4	P	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	8	0	14	1	0
4	R	16	0	28	2	0
4	T	16	0	28	0	0
4	U	8	0	14	1	0
4	V	16	0	28	0	0
4	W	16	0	28	0	0
4	X	8	0	14	1	0
4	Y	8	0	14	1	0
4	Z	8	0	14	0	0
4	a	8	0	14	0	0
4	b	8	0	14	0	0
4	c	24	0	42	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	T	1	0	0	0	0
5	U	1	0	0	0	0
5	V	1	0	0	0	0
5	b	1	0	0	0	0
5	c	1	0	0	0	0
6	A	8	0	0	0	0
6	B	7	0	0	0	0
6	C	3	0	0	0	0
6	D	9	0	0	1	0
6	E	6	0	0	0	0
6	F	6	0	0	0	0
6	G	5	0	0	1	0
6	H	13	0	0	0	0
6	I	6	0	0	0	0
6	J	4	0	0	0	0
6	K	5	0	0	2	0
6	L	3	0	0	0	0
6	M	8	0	0	1	0
6	N	11	0	0	0	0
6	O	9	0	0	0	0
6	P	3	0	0	0	0
6	Q	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	5	0	0	1	0
6	T	7	0	0	1	0
6	U	9	0	0	0	0
6	V	3	0	0	0	0
6	W	1	0	0	0	0
6	X	5	0	0	0	0
6	Y	6	0	0	0	0
6	Z	8	0	0	0	0
6	a	9	0	0	0	0
6	b	7	0	0	0	0
6	c	8	0	0	0	0
All	All	108950	0	112494	984	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (984) 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)
2:D:230:ILE:HG13	2:D:261:THR:HG21	1.29	1.09
1:F:230:ILE:HD11	1:F:261:THR:HB	1.46	0.97
2:D:230:ILE:CG1	2:D:261:THR:HG21	1.95	0.95
1:F:230:ILE:CD1	1:F:261:THR:HB	1.98	0.94
2:Z:230:ILE:HG21	2:Z:261:THR:HG21	1.51	0.93
2:L:131:LEU:HD12	2:L:422:VAL:HG21	1.53	0.88
2:K:222:LEU:O	2:K:301:ILE:HG22	1.73	0.87
2:W:131:LEU:HD12	2:W:422:VAL:HG11	1.57	0.86
2:c:132:LYS:O	3:c:602:BME:H21	1.74	0.86
2:Z:131:LEU:HD12	2:Z:422:VAL:HG21	1.55	0.86
2:Z:269:GLY:HA3	1:a:257:GLU:OE2	1.77	0.84
2:L:222:LEU:CD2	2:L:250:ILE:HD11	2.09	0.82
2:D:222:LEU:CD2	2:D:250:ILE:HD11	2.10	0.82
1:M:131:LEU:HD12	1:M:422:VAL:HG11	1.61	0.82
2:W:349:ILE:HD11	2:W:369:VAL:HG13	1.61	0.82
1:a:131:LEU:HD12	1:a:422:VAL:HG11	1.59	0.82
2:L:239:ALA:HB1	2:L:314:LEU:HD11	1.62	0.81
1:I:131:LEU:HD12	1:I:422:VAL:HG11	1.61	0.81
2:Z:230:ILE:HG21	2:Z:261:THR:CG2	2.10	0.81
1:F:239:ALA:HB1	1:F:314:LEU:HD11	1.63	0.81
2:W:239:ALA:HB1	2:W:314:LEU:HD11	1.62	0.80
1:P:239:ALA:HB1	1:P:314:LEU:HD11	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:239:ALA:HB1	1:b:314:LEU:HD11	1.63	0.80
1:a:239:ALA:HB1	1:a:314:LEU:HD11	1.62	0.79
1:F:220:ILE:HD11	1:F:296:THR:HG21	1.63	0.79
2:K:278:ALA:HB1	2:K:289:LEU:HD21	1.63	0.78
1:G:222:LEU:CD2	1:G:250:ILE:HD11	2.12	0.78
1:F:289:LEU:HD12	1:F:292:ILE:HD11	1.66	0.78
2:W:349:ILE:CD1	2:W:369:VAL:HG13	2.13	0.78
1:A:289:LEU:HD12	1:A:292:ILE:HD11	1.65	0.77
2:E:233:MET:HA	2:E:233:MET:HE2	1.68	0.76
1:N:268:ARG:HH11	1:N:268:ARG:HG2	1.50	0.76
2:Z:131:LEU:CD1	2:Z:422:VAL:HG21	2.17	0.74
1:a:200:LEU:HD21	1:a:277:LYS:HG3	1.69	0.74
1:Q:230:ILE:HG23	1:Q:258:ALA:HA	1.70	0.73
2:D:213:VAL:CG1	2:D:325:ILE:HB	2.19	0.73
1:a:213:VAL:CG1	1:a:325:ILE:HB	2.18	0.73
2:E:239:ALA:HB1	2:E:314:LEU:HD11	1.70	0.73
1:N:268:ARG:HH11	1:N:268:ARG:CG	2.02	0.72
2:L:131:LEU:CD1	2:L:422:VAL:HG21	2.18	0.72
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.72	0.72
2:Z:230:ILE:CG2	2:Z:261:THR:HG21	2.19	0.72
2:L:250:ILE:HG22	2:L:276:VAL:HG13	1.71	0.71
1:a:239:ALA:HB1	1:a:314:LEU:CD1	2.20	0.71
2:Z:213:VAL:CG1	2:Z:325:ILE:HB	2.20	0.71
1:G:213:VAL:CG1	1:G:325:ILE:HB	2.20	0.71
2:W:349:ILE:HD11	2:W:369:VAL:CG1	2.21	0.71
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.73	0.70
2:W:27:VAL:HG12	2:W:90:THR:HG23	1.73	0.70
2:K:220:ILE:HD11	2:K:296:THR:HG21	1.74	0.69
1:U:230:ILE:HG23	1:U:258:ALA:HA	1.71	0.69
2:K:13:ARG:NH1	6:K:701:HOH:O	2.24	0.69
2:K:239:ALA:HB1	2:K:314:LEU:HD11	1.75	0.69
1:b:239:ALA:HB1	1:b:314:LEU:CD1	2.22	0.69
1:b:27:VAL:HG12	1:b:90:THR:HG23	1.74	0.69
2:L:239:ALA:HB1	2:L:314:LEU:CD1	2.23	0.69
1:U:27:VAL:HG12	1:U:90:THR:HG23	1.75	0.69
2:X:205:ILE:HD11	2:X:211:GLY:HA2	1.73	0.69
2:K:301:ILE:HG23	2:K:301:ILE:O	1.93	0.68
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.75	0.68
2:D:230:ILE:HG13	2:D:261:THR:CG2	2.14	0.68
2:L:27:VAL:HG12	2:L:90:THR:HG23	1.75	0.68
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:ALA:HB1	1:F:314:LEU:CD1	2.22	0.68
2:W:296:THR:HG22	2:W:319:GLN:N	2.09	0.68
1:P:239:ALA:HB1	1:P:314:LEU:CD1	2.24	0.67
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.75	0.67
1:J:239:ALA:HB1	1:J:314:LEU:HD11	1.75	0.67
2:W:239:ALA:HB1	2:W:314:LEU:CD1	2.24	0.67
1:G:250:ILE:HG22	1:G:276:VAL:CG2	2.24	0.67
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.75	0.66
2:O:27:VAL:HG12	2:O:90:THR:HG23	1.76	0.66
2:R:77:VAL:HG21	2:R:510:VAL:CG1	2.26	0.66
1:I:131:LEU:CD1	1:I:422:VAL:HG11	2.26	0.66
1:G:296:THR:HG22	1:G:319:GLN:N	2.11	0.66
2:E:239:ALA:HB1	2:E:314:LEU:CD1	2.26	0.66
1:M:82:ASN:HB2	1:M:89:THR:CG2	2.26	0.66
1:a:27:VAL:HG12	1:a:90:THR:HG23	1.77	0.66
1:G:305:ILE:HB	6:G:702:HOH:O	1.96	0.65
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.78	0.65
1:J:242:LYS:O	1:J:243:ALA:HB3	1.95	0.65
2:Z:27:VAL:HG12	2:Z:90:THR:HG23	1.78	0.65
1:A:230:ILE:HD12	1:A:233:MET:SD	2.36	0.65
1:a:200:LEU:HD12	1:a:254:VAL:HG22	1.77	0.65
1:M:131:LEU:CD1	1:M:422:VAL:HG11	2.26	0.65
1:Q:16:MET:SD	1:Q:73:MET:HE1	2.37	0.65
1:Q:133:ALA:HA	3:Q:601:BME:H21	1.78	0.64
2:V:27:VAL:HG12	2:V:90:THR:HG23	1.78	0.64
1:a:131:LEU:CD1	1:a:422:VAL:HG11	2.28	0.64
1:C:296:THR:HG22	1:C:319:GLN:N	2.11	0.64
1:N:77:VAL:HG11	1:N:510:VAL:HG13	1.78	0.64
2:E:213:VAL:HG22	2:E:325:ILE:HB	1.80	0.64
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.80	0.64
2:R:267:MET:HE2	2:R:267:MET:HA	1.79	0.64
2:V:111:MET:HE1	2:V:438:VAL:HB	1.79	0.64
1:A:114:MET:HE2	1:G:36:ARG:HD3	1.80	0.64
1:A:219:PHE:CE2	1:A:245:LYS:HD2	2.32	0.64
1:I:39:VAL:HG21	1:J:16:MET:HE1	1.78	0.64
2:Z:242:LYS:O	2:Z:243:ALA:HB3	1.97	0.64
1:F:39:VAL:HG21	1:G:16:MET:HE1	1.79	0.64
1:B:242:LYS:O	1:B:243:ALA:HB3	1.97	0.63
2:L:230:ILE:HG23	2:L:258:ALA:HA	1.80	0.63
1:C:16:MET:SD	1:C:73:MET:HE1	2.38	0.63
1:J:16:MET:HE2	1:J:73:MET:HE1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ILE:HG23	1:C:301:ILE:O	1.99	0.63
2:L:301:ILE:HG23	2:L:301:ILE:O	1.98	0.63
1:T:305:ILE:HD11	1:T:307:MET:HE3	1.79	0.63
1:b:220:ILE:HD12	1:b:296:THR:HG21	1.78	0.63
2:D:250:ILE:HG22	2:D:276:VAL:CG2	2.28	0.63
1:I:242:LYS:O	1:I:243:ALA:HB3	1.97	0.63
2:L:213:VAL:HG22	2:L:325:ILE:HB	1.80	0.63
2:R:82:ASN:HB2	2:R:89:THR:CG2	2.28	0.63
2:E:340:ALA:HA	2:E:343:GLN:HE21	1.64	0.63
1:F:230:ILE:CD1	1:F:261:THR:CB	2.75	0.63
1:M:82:ASN:HB2	1:M:89:THR:HG23	1.81	0.63
2:Z:77:VAL:HG21	2:Z:510:VAL:CG1	2.29	0.63
2:D:82:ASN:HB2	2:D:89:THR:CG2	2.29	0.62
2:K:239:ALA:HB1	2:K:314:LEU:CD1	2.28	0.62
1:Y:301:ILE:HG23	1:Y:301:ILE:O	1.99	0.62
2:V:229:ASN:HD22	2:V:231:ARG:HG2	1.63	0.62
1:b:16:MET:SD	1:b:73:MET:HE1	2.39	0.62
1:F:36:ARG:HD3	1:G:114:MET:HE2	1.81	0.62
2:R:82:ASN:HB2	2:R:89:THR:HG23	1.79	0.62
2:E:232:GLU:HB2	2:E:309:LEU:HD11	1.81	0.62
1:G:301:ILE:HG23	1:G:301:ILE:O	2.00	0.62
2:O:77:VAL:HG21	2:O:510:VAL:CG1	2.30	0.62
2:D:82:ASN:HB2	2:D:89:THR:HG23	1.82	0.62
1:U:176:THR:HG21	1:U:333:ILE:HD13	1.82	0.62
2:O:114:MET:HE2	1:U:36:ARG:HD3	1.80	0.62
1:B:314:LEU:HD12	1:B:317:LEU:HD13	1.82	0.61
2:Z:176:THR:HG21	2:Z:333:ILE:HD13	1.81	0.61
1:G:220:ILE:HD12	1:G:296:THR:HG21	1.82	0.61
1:T:242:LYS:O	1:T:243:ALA:HB3	2.00	0.61
2:E:506:TYR:CE1	4:E:604:HEZ:H41	2.35	0.61
1:F:292:ILE:O	1:F:296:THR:HG22	2.00	0.61
1:P:27:VAL:HG12	1:P:90:THR:HG23	1.82	0.61
2:X:200:LEU:HD13	2:X:276:VAL:HA	1.81	0.61
2:Z:36:ARG:HD3	1:a:114:MET:HE2	1.82	0.61
2:D:36:ARG:HD3	2:E:114:MET:HE2	1.82	0.61
2:X:82:ASN:HB2	2:X:89:THR:CG2	2.31	0.61
1:J:239:ALA:HB1	1:J:314:LEU:CD1	2.30	0.61
1:I:82:ASN:HB2	1:I:89:THR:CG2	2.30	0.61
2:O:176:THR:HG21	2:O:333:ILE:HD13	1.82	0.61
2:V:220:ILE:HD13	2:V:248:LEU:HD23	1.83	0.61
2:X:242:LYS:O	2:X:243:ALA:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:227:ILE:HD13	2:Z:233:MET:HE1	1.83	0.61
1:A:239:ALA:HB1	1:A:314:LEU:HD11	1.83	0.60
1:G:401:HIS:HB3	3:G:603:BME:H21	1.83	0.60
1:a:230:ILE:HG23	1:a:258:ALA:HA	1.83	0.60
2:D:213:VAL:HG12	2:D:325:ILE:HB	1.83	0.60
2:K:501:ARG:HH12	4:K:602:HEZ:H21	1.65	0.60
1:b:296:THR:HG22	1:b:319:GLN:N	2.15	0.60
1:Q:525:PRO:O	1:Q:526:LYS:C	2.44	0.60
2:V:242:LYS:O	2:V:243:ALA:HB3	1.99	0.60
1:G:213:VAL:HG12	1:G:325:ILE:HB	1.83	0.60
2:R:214:GLU:HG2	2:R:324:VAL:HG12	1.83	0.60
2:c:242:LYS:O	2:c:243:ALA:HB3	2.00	0.60
1:a:16:MET:SD	1:a:73:MET:HE1	2.41	0.60
1:Y:176:THR:HG21	1:Y:333:ILE:HD13	1.82	0.60
2:R:176:THR:HG21	2:R:333:ILE:HD13	1.84	0.60
2:V:176:THR:HG21	2:V:333:ILE:HD13	1.83	0.60
1:N:16:MET:SD	1:N:73:MET:HE1	2.42	0.59
1:N:77:VAL:HG21	1:N:510:VAL:CG1	2.33	0.59
2:W:131:LEU:CD1	2:W:422:VAL:HG11	2.28	0.59
2:R:313:THR:HG23	2:R:315:GLU:HG2	1.85	0.59
1:a:301:ILE:HG23	1:a:301:ILE:O	2.01	0.59
1:b:176:THR:HG21	1:b:333:ILE:HD13	1.85	0.59
2:K:249:ILE:CD1	2:K:254:VAL:HG21	2.32	0.59
1:U:82:ASN:HB2	1:U:89:THR:OG1	2.02	0.59
1:A:176:THR:HG21	1:A:333:ILE:HD13	1.85	0.59
2:W:230:ILE:HG12	2:W:258:ALA:HA	1.85	0.59
1:H:176:THR:HG21	1:H:333:ILE:HD13	1.84	0.59
1:N:77:VAL:HG11	1:N:510:VAL:CG1	2.32	0.59
1:Q:301:ILE:HG21	1:Q:309:LEU:HD23	1.84	0.59
2:Z:230:ILE:HG23	2:Z:258:ALA:HA	1.85	0.59
1:A:220:ILE:HD13	1:A:332:ILE:HD11	1.84	0.59
2:D:242:LYS:O	2:D:243:ALA:HB3	2.02	0.59
2:K:249:ILE:HD11	2:K:254:VAL:HG21	1.83	0.59
2:D:398:ASP:OD1	6:D:701:HOH:O	2.17	0.58
1:a:296:THR:HG22	1:a:319:GLN:N	2.18	0.58
2:K:496:PRO:O	2:K:499:VAL:HG12	2.03	0.58
2:L:294:THR:HG21	2:L:345:ARG:HG2	1.85	0.58
1:M:16:MET:SD	1:M:73:MET:HE1	2.43	0.58
1:T:77:VAL:HG21	1:T:510:VAL:CG1	2.34	0.58
2:D:176:THR:HG21	2:D:333:ILE:HD13	1.85	0.58
1:Y:205:ILE:HD11	1:Y:211:GLY:HA2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:MET:SD	1:I:73:MET:HE1	2.44	0.58
2:X:16:MET:SD	2:X:73:MET:HE1	2.44	0.58
2:c:77:VAL:HG21	2:c:510:VAL:CG1	2.32	0.58
1:B:213:VAL:HG12	1:B:215:LEU:HD11	1.86	0.58
2:E:77:VAL:HG21	2:E:510:VAL:CG1	2.33	0.58
1:G:16:MET:HE3	1:G:520:MET:HE3	1.86	0.58
2:c:82:ASN:HB2	2:c:89:THR:OG1	2.04	0.58
2:L:222:LEU:HD23	2:L:250:ILE:HD11	1.85	0.58
2:Z:16:MET:SD	2:Z:73:MET:HE1	2.44	0.58
2:D:249:ILE:HD11	2:D:275:ALA:HB1	1.86	0.57
1:I:82:ASN:HB2	1:I:89:THR:HG23	1.86	0.57
2:E:242:LYS:O	2:E:243:ALA:HB3	2.04	0.57
2:O:82:ASN:HB2	2:O:89:THR:OG1	2.04	0.57
2:K:249:ILE:HG13	2:K:275:ALA:HA	1.86	0.57
1:N:176:THR:HG21	1:N:333:ILE:HD13	1.86	0.57
1:C:200:LEU:HD13	1:C:276:VAL:HA	1.87	0.57
2:E:49:ILE:HD11	1:F:73:MET:HE3	1.87	0.57
1:N:82:ASN:HB2	1:N:89:THR:OG1	2.05	0.57
1:B:266:THR:CG2	1:B:273:VAL:HG12	2.34	0.57
1:A:227:ILE:HG21	1:A:233:MET:HE3	1.86	0.57
1:F:234:LEU:N	1:F:235:PRO:HD2	2.19	0.57
2:L:16:MET:SD	2:L:73:MET:HE1	2.44	0.57
2:W:421:ARG:NH2	2:W:469:VAL:O	2.37	0.57
1:M:169:VAL:HG21	1:M:377:ALA:HB2	1.86	0.57
2:K:222:LEU:HD23	2:K:250:ILE:CG2	2.34	0.57
1:B:82:ASN:HB2	1:B:89:THR:OG1	2.05	0.56
2:K:227:ILE:HD11	2:K:254:VAL:HG22	1.87	0.56
1:F:200:LEU:HD13	1:F:254:VAL:HG12	1.86	0.56
2:K:249:ILE:C	2:K:249:ILE:HD12	2.29	0.56
1:a:301:ILE:HD13	1:a:309:LEU:HD12	1.87	0.56
1:b:82:ASN:HB2	1:b:89:THR:OG1	2.05	0.56
2:O:16:MET:SD	2:O:73:MET:HE1	2.45	0.56
1:U:230:ILE:HG21	1:U:261:THR:HB	1.87	0.56
2:V:77:VAL:HG21	2:V:510:VAL:CG1	2.36	0.56
2:V:82:ASN:HB2	2:V:89:THR:OG1	2.05	0.56
1:M:336:VAL:HG12	1:M:336:VAL:O	2.06	0.56
2:R:340:ALA:HA	2:R:343:GLN:HE21	1.71	0.56
2:W:234:LEU:N	2:W:235:PRO:HD2	2.21	0.56
2:X:82:ASN:HB2	2:X:89:THR:HG23	1.87	0.56
1:A:239:ALA:HB1	1:A:314:LEU:CD1	2.35	0.56
2:D:220:ILE:HD13	2:D:248:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:MET:SD	1:H:73:MET:HE1	2.46	0.56
2:Z:213:VAL:HG12	2:Z:325:ILE:HB	1.87	0.56
1:P:16:MET:SD	1:P:73:MET:HE1	2.46	0.56
1:N:77:VAL:HG21	1:N:510:VAL:HG13	1.87	0.55
1:T:16:MET:SD	1:T:73:MET:HE1	2.46	0.55
2:c:336:VAL:HG12	2:c:336:VAL:O	2.05	0.55
1:G:176:THR:HG21	1:G:333:ILE:HD13	1.88	0.55
1:P:77:VAL:HG21	1:P:510:VAL:CG1	2.36	0.55
2:X:269:GLY:HA3	1:Y:229:ASN:ND2	2.22	0.55
1:A:234:LEU:N	1:A:235:PRO:HD2	2.21	0.55
1:H:496:PRO:O	1:H:499:VAL:HG12	2.06	0.55
2:K:203:TYR:HD2	2:K:267:MET:HE3	1.71	0.55
2:O:239:ALA:HB1	2:O:314:LEU:CD1	2.36	0.55
1:H:336:VAL:HG12	1:H:336:VAL:O	2.05	0.55
2:O:336:VAL:HG12	2:O:336:VAL:O	2.06	0.55
2:V:114:MET:HE2	1:b:36:ARG:HD3	1.88	0.55
1:N:305:ILE:HD11	1:N:307:MET:HE3	1.89	0.55
2:V:16:MET:SD	2:V:73:MET:HE1	2.47	0.55
1:H:82:ASN:HB2	1:H:89:THR:OG1	2.06	0.55
2:D:249:ILE:HD13	2:D:254:VAL:HG21	1.87	0.55
1:F:176:THR:HG21	1:F:333:ILE:HD13	1.88	0.55
1:I:336:VAL:HG12	1:I:336:VAL:O	2.06	0.55
2:K:234:LEU:N	2:K:235:PRO:HD2	2.22	0.55
1:Y:36:ARG:HD3	2:Z:114:MET:HE2	1.88	0.55
1:F:77:VAL:HG21	1:F:510:VAL:CG1	2.37	0.55
2:L:301:ILE:HD13	2:L:309:LEU:HD12	1.88	0.55
1:a:200:LEU:CD1	1:a:254:VAL:HG22	2.36	0.55
1:b:187:LEU:C	1:b:187:LEU:HD23	2.31	0.55
1:B:336:VAL:HG12	1:B:336:VAL:O	2.07	0.55
1:Y:16:MET:SD	1:Y:73:MET:HE1	2.46	0.55
1:Y:225:LYS:NZ	1:Y:232:GLU:OE2	2.37	0.55
2:E:232:GLU:HB2	2:E:309:LEU:CD1	2.36	0.54
1:H:114:MET:HE2	1:N:36:ARG:HD3	1.88	0.54
1:J:16:MET:HE2	1:J:73:MET:CE	2.37	0.54
2:L:77:VAL:HG21	2:L:510:VAL:CG1	2.37	0.54
1:Q:193:MET:HG3	1:Q:371:LYS:HB3	1.90	0.54
1:Q:234:LEU:N	1:Q:235:PRO:HD2	2.22	0.54
2:W:220:ILE:HD12	2:W:296:THR:HG21	1.89	0.54
1:H:187:LEU:HD23	1:H:187:LEU:C	2.33	0.54
2:K:278:ALA:CB	2:K:289:LEU:HD21	2.34	0.54
2:Z:269:GLY:O	2:Z:270:ILE:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:230:ILE:HG21	1:a:261:THR:OG1	2.06	0.54
2:D:222:LEU:HD23	2:D:250:ILE:HD11	1.90	0.54
1:H:77:VAL:HG21	1:H:510:VAL:CG1	2.36	0.54
2:K:88:GLY:HA2	2:K:91:THR:HG22	1.90	0.54
2:W:82:ASN:HB2	2:W:89:THR:OG1	2.07	0.54
1:I:234:LEU:N	1:I:235:PRO:HD2	2.23	0.54
1:P:336:VAL:HG12	1:P:336:VAL:O	2.08	0.54
1:Y:349:ILE:CG2	1:Y:369:VAL:HG22	2.38	0.54
2:Z:82:ASN:HB2	2:Z:89:THR:OG1	2.08	0.54
1:A:82:ASN:HB2	1:A:89:THR:OG1	2.08	0.54
1:C:525:PRO:O	1:C:526:LYS:C	2.51	0.54
2:D:234:LEU:N	2:D:235:PRO:HD2	2.22	0.54
2:E:234:LEU:N	2:E:235:PRO:HD2	2.22	0.54
1:F:230:ILE:HG13	1:F:258:ALA:HA	1.88	0.54
1:Q:77:VAL:HG21	1:Q:510:VAL:CG1	2.38	0.54
2:Z:130:GLU:HB3	2:Z:422:VAL:HG22	1.90	0.54
2:X:230:ILE:N	2:X:230:ILE:HD12	2.22	0.54
2:V:336:VAL:O	2:V:336:VAL:HG12	2.07	0.54
2:X:343:GLN:HA	2:X:346:VAL:HG22	1.90	0.54
1:Y:234:LEU:N	1:Y:235:PRO:HD2	2.23	0.54
1:U:234:LEU:N	1:U:235:PRO:HD2	2.23	0.54
2:K:225:LYS:HE2	2:K:303:GLU:HB2	1.90	0.53
3:M:601:BME:H21	1:N:518:GLU:HG3	1.90	0.53
2:V:234:LEU:N	2:V:235:PRO:HD2	2.22	0.53
2:c:234:LEU:N	2:c:235:PRO:HD2	2.23	0.53
1:H:234:LEU:N	1:H:235:PRO:HD2	2.23	0.53
2:L:269:GLY:HA3	1:M:229:ASN:CG	2.32	0.53
1:N:234:LEU:N	1:N:235:PRO:HD2	2.22	0.53
1:N:268:ARG:CG	1:N:268:ARG:NH1	2.69	0.53
2:V:220:ILE:HD11	2:V:250:ILE:HG13	1.90	0.53
1:Q:445:ARG:HB2	3:Q:603:BME:S2	2.49	0.53
2:Z:336:VAL:HG12	2:Z:336:VAL:O	2.09	0.53
2:K:292:ILE:O	2:K:296:THR:HG22	2.09	0.53
1:P:385:THR:HG22	1:P:387:VAL:H	1.74	0.53
1:U:16:MET:SD	1:U:73:MET:HE1	2.48	0.53
1:Y:349:ILE:HG23	1:Y:369:VAL:HG22	1.91	0.53
2:Z:230:ILE:CG2	2:Z:261:THR:CG2	2.83	0.53
2:Z:234:LEU:N	2:Z:235:PRO:HD2	2.23	0.53
1:a:234:LEU:N	1:a:235:PRO:HD2	2.23	0.53
1:P:234:LEU:N	1:P:235:PRO:HD2	2.23	0.53
1:B:234:LEU:N	1:B:235:PRO:HD2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:MET:HB3	1:G:514:MET:HE3	1.90	0.53
1:J:242:LYS:O	1:J:243:ALA:CB	2.56	0.53
2:L:234:LEU:N	2:L:235:PRO:HD2	2.23	0.53
2:V:266:THR:CG2	2:V:273:VAL:HG12	2.38	0.53
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.09	0.53
2:K:82:ASN:HB2	2:K:89:THR:OG1	2.08	0.53
2:R:36:ARG:HD3	2:c:114:MET:HE2	1.91	0.53
1:A:16:MET:SD	1:A:73:MET:HE1	2.49	0.52
1:H:114:MET:HB3	1:H:118:ARG:HH12	1.74	0.52
2:O:234:LEU:N	2:O:235:PRO:HD2	2.24	0.52
1:T:234:LEU:N	1:T:235:PRO:HD2	2.23	0.52
1:F:200:LEU:CD1	1:F:254:VAL:HG12	2.38	0.52
1:F:220:ILE:CD1	1:F:296:THR:HG21	2.35	0.52
1:G:250:ILE:HG22	1:G:276:VAL:HG23	1.91	0.52
2:L:496:PRO:O	2:L:499:VAL:HG22	2.10	0.52
1:Q:135:SER:O	3:Q:601:BME:S2	2.67	0.52
2:X:214:GLU:OE2	2:X:322:ARG:NH2	2.43	0.52
1:A:213:VAL:HG12	1:A:215:LEU:HD11	1.90	0.52
1:U:305:ILE:HD11	1:U:307:MET:HE3	1.91	0.52
2:c:16:MET:SD	2:c:73:MET:HE1	2.49	0.52
2:X:230:ILE:HD11	2:X:257:GLU:HG3	1.91	0.52
2:E:16:MET:SD	2:E:73:MET:HE1	2.49	0.52
1:G:234:LEU:N	1:G:235:PRO:HD2	2.25	0.52
2:V:215:LEU:HB2	2:V:323:VAL:HG22	1.91	0.52
1:J:234:LEU:N	1:J:235:PRO:HD2	2.25	0.52
1:F:82:ASN:HB2	1:F:89:THR:OG1	2.10	0.52
1:N:187:LEU:C	1:N:187:LEU:HD23	2.35	0.52
2:E:296:THR:HG23	2:E:318:GLY:HA3	1.92	0.52
2:X:176:THR:HG21	2:X:333:ILE:HD13	1.91	0.52
1:C:234:LEU:N	1:C:235:PRO:HD2	2.25	0.52
1:G:200:LEU:CD1	1:G:254:VAL:HG12	2.39	0.52
1:J:203:TYR:HB3	1:J:267:MET:HE2	1.91	0.52
1:Y:165:ALA:HB2	1:Y:379:ILE:HD11	1.92	0.52
1:a:222:LEU:N	1:a:222:LEU:HD22	2.25	0.52
1:C:114:MET:HB3	1:C:118:ARG:HH12	1.75	0.52
1:T:114:MET:HE2	2:c:36:ARG:HD3	1.92	0.52
1:C:213:VAL:HG12	1:C:215:LEU:HD11	1.91	0.51
2:K:16:MET:SD	2:K:73:MET:HE1	2.50	0.51
1:T:18:ARG:HG3	6:T:706:HOH:O	2.11	0.51
1:C:417:VAL:HG21	1:C:488:MET:HG3	1.92	0.51
1:Q:417:VAL:HG21	1:Q:488:MET:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:496:PRO:O	2:V:499:VAL:HG22	2.10	0.51
1:a:225:LYS:HG2	1:a:226:LYS:N	2.24	0.51
1:A:187:LEU:C	1:A:187:LEU:HD23	2.35	0.51
1:G:249:ILE:HD11	1:G:275:ALA:HB1	1.91	0.51
1:P:305:ILE:O	1:P:305:ILE:HG22	2.09	0.51
1:a:345:ARG:O	1:a:349:ILE:HG12	2.10	0.51
1:J:16:MET:HB3	1:J:514:MET:HE3	1.93	0.51
1:M:200:LEU:HD13	1:M:276:VAL:HA	1.91	0.51
1:N:165:ALA:HA	1:N:187:LEU:HD11	1.92	0.51
1:T:82:ASN:HB2	1:T:89:THR:OG1	2.11	0.51
2:V:49:ILE:HD11	2:W:73:MET:HE3	1.92	0.51
2:E:82:ASN:HB2	2:E:89:THR:OG1	2.11	0.51
2:W:266:THR:CG2	2:W:273:VAL:HG12	2.40	0.51
2:E:36:ARG:HD3	1:F:114:MET:HE2	1.93	0.51
2:R:234:LEU:N	2:R:235:PRO:HD2	2.26	0.51
2:X:234:LEU:N	2:X:235:PRO:HD2	2.25	0.51
2:Z:157:THR:O	2:Z:161:LEU:HD23	2.10	0.51
1:a:213:VAL:HG12	1:a:325:ILE:HB	1.90	0.51
1:A:336:VAL:HG12	1:A:336:VAL:O	2.11	0.51
2:L:193:MET:HG3	2:L:371:LYS:HB3	1.92	0.51
1:Q:230:ILE:HG21	1:Q:261:THR:HB	1.92	0.51
2:Z:85:ALA:HB1	2:Z:499:VAL:HG12	1.92	0.51
1:M:166:MET:HE2	1:M:171:LYS:HA	1.93	0.51
1:M:234:LEU:N	1:M:235:PRO:HD2	2.26	0.51
1:A:220:ILE:CD1	1:A:332:ILE:HD11	2.41	0.51
1:F:261:THR:HA	1:F:264:VAL:HG22	1.91	0.51
2:K:301:ILE:O	2:K:301:ILE:CG2	2.59	0.51
2:Z:496:PRO:O	2:Z:499:VAL:HG22	2.10	0.51
2:D:16:MET:SD	2:D:73:MET:HE1	2.51	0.50
1:J:176:THR:HG21	1:J:333:ILE:HD13	1.94	0.50
2:L:82:ASN:HB2	2:L:89:THR:OG1	2.11	0.50
2:Z:269:GLY:HA3	1:a:257:GLU:CD	2.34	0.50
1:G:200:LEU:HD13	1:G:254:VAL:HG12	1.92	0.50
1:J:82:ASN:HB2	1:J:89:THR:OG1	2.12	0.50
2:E:305:ILE:HD11	2:E:307:MET:HE3	1.93	0.50
1:F:353:ILE:HG23	1:F:362:ARG:HG2	1.93	0.50
2:O:239:ALA:HB1	2:O:314:LEU:HD11	1.92	0.50
1:Y:85:ALA:HB1	1:Y:499:VAL:HG12	1.94	0.50
1:a:206:ASN:O	1:a:208:PRO:HD3	2.12	0.50
1:B:213:VAL:HG12	1:B:215:LEU:CD1	2.41	0.50
1:b:234:LEU:N	1:b:235:PRO:HD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:ILE:HG22	2:D:276:VAL:HG23	1.93	0.50
1:N:215:LEU:HB2	1:N:323:VAL:HG22	1.94	0.50
2:O:42:LYS:O	2:O:43:SER:C	2.54	0.50
1:Q:62:LEU:H	1:Q:68:ASN:HD22	1.58	0.50
1:Y:205:ILE:CD1	1:Y:211:GLY:HA2	2.42	0.50
2:D:249:ILE:CD1	2:D:254:VAL:HG21	2.42	0.50
2:L:230:ILE:HG21	2:L:261:THR:OG1	2.11	0.50
1:Q:305:ILE:HD11	1:Q:307:MET:HE3	1.94	0.50
1:U:301:ILE:HG21	1:U:309:LEU:HD12	1.94	0.50
2:L:130:GLU:HB3	2:L:422:VAL:HG22	1.94	0.49
2:X:215:LEU:HB2	2:X:323:VAL:HG22	1.94	0.49
1:I:524:LEU:HD23	1:I:525:PRO:HD2	1.92	0.49
1:M:220:ILE:HD13	1:M:296:THR:HG21	1.94	0.49
1:P:82:ASN:HB2	1:P:89:THR:OG1	2.11	0.49
2:R:16:MET:SD	2:R:73:MET:HE1	2.52	0.49
2:V:186:GLU:HB2	2:V:380:LYS:HB2	1.94	0.49
2:W:336:VAL:HG12	2:W:336:VAL:O	2.12	0.49
1:Y:82:ASN:HB2	1:Y:89:THR:OG1	2.12	0.49
1:C:215:LEU:HB2	1:C:323:VAL:HG22	1.93	0.49
1:G:17:LEU:HA	1:G:20:VAL:HG12	1.95	0.49
1:J:16:MET:HE3	1:J:520:MET:HE3	1.93	0.49
2:X:230:ILE:HG22	2:X:234:LEU:CD1	2.42	0.49
1:a:169:VAL:HG21	1:a:377:ALA:HB2	1.95	0.49
2:c:266:THR:HG23	2:c:272:LYS:HD2	1.94	0.49
2:D:249:ILE:C	2:D:249:ILE:HD12	2.37	0.49
1:H:215:LEU:HB2	1:H:323:VAL:HG22	1.93	0.49
2:L:221:LEU:HD23	2:L:249:ILE:HD12	1.94	0.49
1:Y:215:LEU:HB2	1:Y:323:VAL:HG22	1.94	0.49
2:K:203:TYR:CD2	2:K:267:MET:HE3	2.47	0.49
2:K:249:ILE:HD12	2:K:249:ILE:O	2.13	0.49
2:L:16:MET:HB3	2:L:514:MET:HE3	1.95	0.49
1:Q:268:ARG:O	2:R:229:ASN:ND2	2.46	0.49
1:B:242:LYS:O	1:B:243:ALA:CB	2.61	0.49
1:G:249:ILE:HG13	1:G:275:ALA:HA	1.94	0.49
1:I:242:LYS:O	1:I:243:ALA:CB	2.60	0.49
2:V:85:ALA:HB1	2:V:499:VAL:HG12	1.93	0.49
1:Y:496:PRO:O	1:Y:499:VAL:HG22	2.11	0.49
2:Z:242:LYS:O	2:Z:243:ALA:CB	2.61	0.49
2:K:449:ALA:HB3	2:K:450:PRO:HD3	1.95	0.49
2:R:324:VAL:HG22	2:R:331:THR:CG2	2.42	0.49
1:H:305:ILE:HD11	1:H:307:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:385:THR:HG22	2:R:387:VAL:H	1.77	0.49
1:A:239:ALA:HA	1:A:242:LYS:HD3	1.95	0.49
2:L:250:ILE:HG22	2:L:276:VAL:CG1	2.40	0.49
2:D:230:ILE:HG12	2:D:261:THR:HG21	1.89	0.49
2:K:230:ILE:HG12	2:K:258:ALA:HA	1.93	0.49
1:M:186:GLU:HB2	1:M:380:LYS:HB2	1.95	0.48
2:Z:346:VAL:HG13	2:Z:369:VAL:HG13	1.95	0.48
1:b:525:PRO:O	1:b:526:LYS:C	2.55	0.48
1:B:280:GLY:HA2	4:B:604:HEZ:C1	2.43	0.48
1:G:11:ASP:O	1:G:15:LYS:HG2	2.12	0.48
1:B:266:THR:HG23	1:B:273:VAL:HG12	1.96	0.48
1:I:215:LEU:HB2	1:I:323:VAL:HG22	1.94	0.48
1:J:270:ILE:HG13	2:K:231:ARG:HH12	1.79	0.48
1:Q:215:LEU:HB2	1:Q:323:VAL:HG22	1.94	0.48
1:H:165:ALA:HA	1:H:187:LEU:HD11	1.95	0.48
2:K:222:LEU:HD13	2:K:293:ALA:HB2	1.94	0.48
1:Q:61:GLU:HG3	1:Q:68:ASN:HD21	1.79	0.48
1:G:193:MET:HG3	1:G:371:LYS:HB3	1.95	0.48
2:K:200:LEU:HD21	2:K:277:LYS:HG3	1.95	0.48
2:K:221:LEU:HD21	2:K:249:ILE:HG22	1.94	0.48
2:L:393:LYS:NZ	2:L:397:GLU:OE1	2.46	0.48
1:T:295:LEU:HD13	1:T:295:LEU:C	2.38	0.48
2:Z:269:GLY:CA	1:a:257:GLU:OE2	2.58	0.48
1:a:82:ASN:HB2	1:a:89:THR:OG1	2.13	0.48
1:A:144:ILE:HD13	1:A:166:MET:HE3	1.94	0.48
1:C:16:MET:HB3	1:C:514:MET:HE3	1.95	0.48
1:J:215:LEU:HB2	1:J:323:VAL:HG22	1.95	0.48
2:X:301:ILE:HG23	2:X:301:ILE:O	2.13	0.48
1:Y:227:ILE:HD11	1:Y:254:VAL:HG22	1.95	0.48
2:V:111:MET:HE2	2:V:116:LEU:HD21	1.94	0.48
1:Y:193:MET:HG3	1:Y:371:LYS:HB3	1.96	0.48
1:a:301:ILE:HD11	1:a:308:GLU:O	2.14	0.48
2:K:215:LEU:HB2	2:K:323:VAL:HG22	1.96	0.48
2:O:449:ALA:HB3	2:O:450:PRO:HD3	1.96	0.48
2:R:193:MET:HG3	2:R:371:LYS:HB3	1.95	0.48
2:R:449:ALA:HB3	2:R:450:PRO:HD3	1.96	0.48
2:D:257:GLU:O	2:D:261:THR:HG22	2.14	0.48
1:H:16:MET:HB3	1:H:514:MET:HE3	1.96	0.48
1:I:295:LEU:C	1:I:295:LEU:HD13	2.39	0.48
2:K:36:ARG:HD3	2:L:114:MET:HE1	1.96	0.48
2:K:249:ILE:HD11	2:K:275:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:198:GLY:O	2:L:276:VAL:HG23	2.14	0.48
2:X:186:GLU:HB2	2:X:380:LYS:HB2	1.96	0.48
1:b:77:VAL:HG21	1:b:510:VAL:CG1	2.43	0.48
2:L:186:GLU:HB2	2:L:380:LYS:HB2	1.95	0.47
1:P:186:GLU:HB2	1:P:380:LYS:HB2	1.95	0.47
2:V:242:LYS:O	2:V:243:ALA:CB	2.62	0.47
1:a:220:ILE:HD12	1:a:222:LEU:HD11	1.96	0.47
1:b:165:ALA:HA	1:b:187:LEU:HD11	1.96	0.47
2:E:409:GLU:HA	3:E:602:BME:H12	1.96	0.47
2:R:77:VAL:HG21	2:R:510:VAL:HG12	1.95	0.47
2:Z:176:THR:CG2	2:Z:322:ARG:HH21	2.27	0.47
2:E:16:MET:HB3	2:E:514:MET:HE3	1.95	0.47
1:M:43:SEP:O1P	1:M:43:SEP:HA	2.14	0.47
1:C:193:MET:HG3	1:C:371:LYS:HB3	1.95	0.47
2:K:91:THR:HG23	2:K:503:ALA:HB1	1.96	0.47
1:M:350:ARG:NE	6:M:701:HOH:O	2.47	0.47
2:O:319:GLN:HG3	2:O:336:VAL:HG21	1.96	0.47
1:F:352:GLN:HA	1:F:355:GLU:HG2	1.95	0.47
2:D:230:ILE:CG1	2:D:261:THR:CG2	2.80	0.47
1:U:16:MET:HB3	1:U:514:MET:HE3	1.97	0.47
2:V:220:ILE:HD11	2:V:250:ILE:CD1	2.44	0.47
2:V:292:ILE:O	2:V:296:THR:HG22	2.14	0.47
1:B:248:LEU:HD13	1:B:325:ILE:HD11	1.95	0.47
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.97	0.47
1:C:82:ASN:HB2	1:C:89:THR:OG1	2.15	0.47
1:G:314:LEU:HA	1:G:317:LEU:CD1	2.45	0.47
1:N:5:ASP:HB2	1:N:524:LEU:HD23	1.96	0.47
2:O:166:MET:HE2	2:O:171:LYS:HA	1.96	0.47
2:R:77:VAL:CG2	2:R:510:VAL:CG1	2.92	0.47
2:R:220:ILE:HD11	2:R:250:ILE:HD12	1.97	0.47
2:W:295:LEU:C	2:W:295:LEU:HD13	2.40	0.47
2:W:348:GLN:O	2:W:351:GLN:HB3	2.14	0.47
2:W:383:ALA:HB3	2:W:389:MET:HB3	1.95	0.47
2:X:242:LYS:O	2:X:243:ALA:CB	2.63	0.47
1:Y:139:SER:O	1:Y:171:LYS:NZ	2.39	0.47
1:b:42:LYS:NZ	1:b:46:ALA:O	2.48	0.47
1:B:16:MET:HB3	1:B:514:MET:HE3	1.97	0.47
2:O:29:VAL:HG12	3:O:602:BME:H22	1.97	0.47
2:Z:16:MET:HB3	2:Z:514:MET:HE3	1.97	0.47
2:K:248:LEU:HD13	2:K:325:ILE:HD11	1.96	0.47
1:M:187:LEU:HD13	1:M:187:LEU:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:205:ILE:HD11	1:Y:208:PRO:HA	1.97	0.47
1:a:305:ILE:O	1:a:305:ILE:HG22	2.15	0.47
2:D:249:ILE:HD12	2:D:249:ILE:O	2.15	0.46
1:F:305:ILE:O	1:F:305:ILE:HG22	2.15	0.46
1:Q:339:GLU:HG2	1:Q:343:GLN:OE1	2.15	0.46
2:W:262:LEU:O	2:W:266:THR:HG23	2.16	0.46
2:c:525:PRO:O	2:c:526:LYS:C	2.58	0.46
1:B:280:GLY:HA2	4:B:604:HEZ:H12	1.98	0.46
1:F:237:LEU:C	1:F:237:LEU:HD12	2.40	0.46
1:Y:449:ALA:HB3	1:Y:450:PRO:HD3	1.98	0.46
1:a:201:SER:HB3	1:a:204:PHE:CD2	2.51	0.46
1:C:220:ILE:HD12	1:C:296:THR:CG2	2.45	0.46
1:J:248:LEU:HD13	1:J:325:ILE:HD11	1.96	0.46
2:K:227:ILE:CG1	2:K:254:VAL:HG22	2.45	0.46
2:K:250:ILE:HG23	2:K:250:ILE:O	2.15	0.46
2:L:352:GLN:HA	2:L:355:GLU:HG2	1.98	0.46
1:P:193:MET:HG3	1:P:371:LYS:HB3	1.97	0.46
2:X:16:MET:HB3	2:X:514:MET:HE3	1.97	0.46
1:Y:249:ILE:HD11	1:Y:275:ALA:HB2	1.96	0.46
1:a:17:LEU:HA	1:a:20:VAL:HG12	1.97	0.46
2:K:183:LEU:O	2:K:183:LEU:HD23	2.16	0.46
1:Q:82:ASN:HB2	1:Q:89:THR:OG1	2.16	0.46
1:U:186:GLU:HB2	1:U:380:LYS:HB2	1.97	0.46
1:U:200:LEU:HD21	1:U:277:LYS:HG3	1.97	0.46
1:a:220:ILE:CD1	1:a:222:LEU:HD21	2.46	0.46
2:D:249:ILE:HG13	2:D:275:ALA:HA	1.96	0.46
2:K:305:ILE:O	2:K:305:ILE:HG22	2.15	0.46
2:K:352:GLN:HA	2:K:355:GLU:HG2	1.98	0.46
1:T:166:MET:HE2	1:T:171:LYS:HA	1.97	0.46
1:U:114:MET:HB3	1:U:118:ARG:HH12	1.80	0.46
2:O:146:GLN:O	2:O:150:ILE:HG12	2.15	0.46
1:Q:16:MET:HB3	1:Q:514:MET:HE3	1.97	0.46
2:V:220:ILE:HG22	2:V:318:GLY:C	2.40	0.46
1:a:449:ALA:HB3	1:a:450:PRO:HD3	1.98	0.46
1:C:227:ILE:HB	1:C:254:VAL:HG12	1.96	0.46
1:C:270:ILE:HD12	2:D:231:ARG:HD2	1.98	0.46
2:D:16:MET:HB3	2:D:514:MET:HE3	1.98	0.46
2:K:221:LEU:HD12	2:K:221:LEU:O	2.16	0.46
2:L:85:ALA:HB1	2:L:499:VAL:HG12	1.97	0.46
1:Y:220:ILE:HD12	1:Y:248:LEU:HD23	1.97	0.46
1:b:260:ALA:O	1:b:263:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.96	0.46
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.98	0.46
1:M:248:LEU:HD13	1:M:325:ILE:HD11	1.98	0.46
1:C:213:VAL:HG12	1:C:215:LEU:CD1	2.46	0.46
1:F:295:LEU:C	1:F:295:LEU:HD13	2.41	0.46
2:K:193:MET:HE3	2:K:292:ILE:HG12	1.98	0.46
2:K:220:ILE:C	2:K:220:ILE:HD12	2.41	0.46
1:P:501:ARG:HH12	4:P:603:HEZ:H12	1.79	0.46
1:T:16:MET:HB3	1:T:514:MET:HE3	1.98	0.46
2:V:193:MET:HG3	2:V:371:LYS:HB3	1.97	0.46
2:X:449:ALA:HB3	2:X:450:PRO:HD3	1.98	0.46
1:A:350:ARG:O	1:A:353:ILE:HG22	2.16	0.46
2:D:259:LEU:C	2:D:259:LEU:HD23	2.41	0.46
1:J:193:MET:HG3	1:J:371:LYS:HB3	1.97	0.46
2:L:215:LEU:HB2	2:L:323:VAL:HG22	1.98	0.46
2:V:111:MET:CE	2:V:116:LEU:HD21	2.46	0.46
2:V:206:ASN:HD22	2:V:272:LYS:CE	2.29	0.46
2:c:242:LYS:O	2:c:243:ALA:CB	2.63	0.46
2:c:305:ILE:HD11	2:c:307:MET:HE3	1.98	0.46
2:W:16:MET:HB3	2:W:514:MET:HE3	1.99	0.45
2:W:217:SER:N	2:W:218:PRO:HD3	2.31	0.45
1:P:199:TYR:CE2	1:P:205:ILE:HD11	2.52	0.45
1:P:305:ILE:O	1:P:305:ILE:CG2	2.64	0.45
1:U:176:THR:CG2	1:U:322:ARG:HH21	2.30	0.45
1:U:449:ALA:HB3	1:U:450:PRO:HD3	1.99	0.45
2:X:269:GLY:HA3	1:Y:229:ASN:HD21	1.82	0.45
2:c:193:MET:HG3	2:c:371:LYS:HB3	1.98	0.45
2:D:183:LEU:O	2:D:183:LEU:HD23	2.16	0.45
2:E:449:ALA:HB3	2:E:450:PRO:HD3	1.98	0.45
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.97	0.45
2:W:186:GLU:HB2	2:W:380:LYS:HB2	1.97	0.45
2:D:215:LEU:HB2	2:D:323:VAL:HG22	1.98	0.45
2:K:193:MET:HG3	2:K:371:LYS:HB3	1.98	0.45
1:T:352:GLN:HA	1:T:355:GLU:HG2	1.98	0.45
2:K:222:LEU:HB2	2:K:300:VAL:HA	1.98	0.45
1:T:248:LEU:HD13	1:T:325:ILE:HD11	1.98	0.45
2:V:16:MET:HB3	2:V:514:MET:HE3	1.98	0.45
1:Y:16:MET:HB3	1:Y:514:MET:HE3	1.98	0.45
1:b:220:ILE:HD12	1:b:296:THR:CG2	2.45	0.45
1:B:16:MET:SD	1:B:73:MET:HE1	2.57	0.45
1:G:222:LEU:HD23	1:G:250:ILE:HD11	1.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:217:SER:N	2:K:218:PRO:HD3	2.32	0.45
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.98	0.45
1:b:186:GLU:HB2	1:b:380:LYS:HB2	1.98	0.45
1:G:222:LEU:O	1:G:301:ILE:HG22	2.17	0.45
2:K:250:ILE:HD12	2:K:276:VAL:HG13	1.98	0.45
2:L:222:LEU:O	2:L:301:ILE:HG22	2.17	0.45
2:X:501:ARG:HH12	4:X:603:HEZ:H62	1.82	0.45
1:a:269:GLY:HA3	1:b:229:ASN:CG	2.41	0.45
1:H:186:GLU:HB2	1:H:380:LYS:HB2	1.98	0.45
2:X:449:ALA:N	2:X:450:PRO:CD	2.80	0.45
1:b:215:LEU:HB2	1:b:323:VAL:HG22	1.99	0.45
2:E:449:ALA:N	2:E:450:PRO:CD	2.80	0.45
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.98	0.45
1:H:353:ILE:HG23	1:H:362:ARG:HG2	1.98	0.45
1:J:186:GLU:HB2	1:J:380:LYS:HB2	1.98	0.45
2:R:246:PRO:HB3	2:R:272:LYS:HG3	1.99	0.45
1:Y:5:ASP:HB2	1:Y:524:LEU:HD23	1.99	0.45
1:a:193:MET:HG3	1:a:371:LYS:HB3	1.98	0.45
1:A:17:LEU:HA	1:A:20:VAL:HG22	1.98	0.45
1:A:248:LEU:HD13	1:A:325:ILE:HD11	1.99	0.45
2:D:305:ILE:O	2:D:305:ILE:HG22	2.17	0.45
1:J:16:MET:CE	1:J:73:MET:HE1	2.46	0.45
1:P:206:ASN:O	1:P:208:PRO:HD3	2.17	0.45
1:P:248:LEU:HD13	1:P:325:ILE:HD11	1.99	0.45
2:c:248:LEU:HD13	2:c:325:ILE:HD11	1.99	0.45
1:A:144:ILE:HG21	1:A:166:MET:CE	2.47	0.44
2:D:186:GLU:HB2	2:D:380:LYS:HB2	1.98	0.44
2:K:353:ILE:CD1	2:K:365:LEU:HB2	2.47	0.44
1:M:220:ILE:HD11	1:M:296:THR:OG1	2.17	0.44
1:N:525:PRO:O	1:N:526:LYS:C	2.61	0.44
1:Y:506:TYR:CZ	4:Y:602:HEZ:H22	2.53	0.44
1:a:201:SER:C	1:a:203:TYR:H	2.26	0.44
2:E:248:LEU:HD13	2:E:325:ILE:HD11	1.98	0.44
1:I:449:ALA:N	1:I:450:PRO:CD	2.80	0.44
2:R:501:ARG:HH12	4:R:603:HEZ:H11	1.81	0.44
2:V:38:VAL:HG12	2:V:40:LEU:CD1	2.48	0.44
1:F:301:ILE:HG21	1:F:309:LEU:HD12	1.97	0.44
1:I:186:GLU:HB2	1:I:380:LYS:HB2	2.00	0.44
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.99	0.44
1:P:200:LEU:HD21	1:P:277:LYS:HG3	2.00	0.44
1:Q:200:LEU:HD21	1:Q:277:LYS:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:183:LEU:HD13	1:Y:183:LEU:C	2.42	0.44
2:Z:36:ARG:HD3	1:a:114:MET:CE	2.45	0.44
1:A:16:MET:HB3	1:A:514:MET:HE3	1.98	0.44
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.98	0.44
1:H:449:ALA:N	1:H:450:PRO:CD	2.81	0.44
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.99	0.44
1:M:42:LYS:O	1:M:43:SEP:C	2.64	0.44
2:O:77:VAL:HG21	2:O:510:VAL:HG12	2.00	0.44
2:Z:248:LEU:HD13	2:Z:325:ILE:HD11	2.00	0.44
1:B:221:LEU:CD2	1:B:233:MET:HE1	2.47	0.44
1:H:14:VAL:O	1:H:18:ARG:HG3	2.17	0.44
2:D:313:THR:OG1	2:D:314:LEU:N	2.51	0.44
2:D:321:LYS:HB3	2:D:334:ASP:HB3	2.00	0.44
1:G:345:ARG:O	1:G:349:ILE:HG12	2.17	0.44
2:K:29:VAL:HG12	3:K:601:BME:H12	2.00	0.44
2:O:16:MET:HB3	2:O:514:MET:HE3	1.99	0.44
2:W:225:LYS:HG2	2:W:226:LYS:N	2.33	0.44
2:W:266:THR:HG22	2:W:273:VAL:H	1.82	0.44
2:X:295:LEU:HD13	2:X:295:LEU:C	2.42	0.44
1:a:342:ILE:HG13	1:a:343:GLN:N	2.33	0.44
1:A:230:ILE:HD13	1:A:261:THR:OG1	2.18	0.44
1:J:16:MET:HE3	1:J:520:MET:SD	2.57	0.44
1:M:5:ASP:HB2	1:M:524:LEU:HD12	2.00	0.44
1:Q:220:ILE:HD12	1:Q:319:GLN:HA	2.00	0.44
1:T:353:ILE:HG23	1:T:362:ARG:HG2	1.98	0.44
2:Z:233:MET:O	2:Z:236:VAL:HG12	2.18	0.44
2:Z:353:ILE:HG23	2:Z:362:ARG:HG2	2.00	0.44
1:b:248:LEU:HD13	1:b:325:ILE:HD11	2.00	0.44
2:D:449:ALA:HB3	2:D:450:PRO:HD3	1.99	0.44
1:G:169:VAL:HG21	1:G:377:ALA:HB2	1.99	0.44
1:M:259:LEU:C	1:M:259:LEU:HD23	2.43	0.44
1:N:449:ALA:N	1:N:450:PRO:CD	2.80	0.44
2:R:271:VAL:HG12	2:R:273:VAL:HG23	2.00	0.44
1:U:193:MET:HG3	1:U:371:LYS:HB3	1.99	0.44
1:Y:248:LEU:HD13	1:Y:325:ILE:HD11	1.99	0.44
1:B:220:ILE:HD12	1:B:248:LEU:HD23	2.00	0.44
1:C:259:LEU:C	1:C:259:LEU:HD23	2.43	0.44
1:G:259:LEU:HD23	1:G:259:LEU:C	2.43	0.44
1:M:220:ILE:O	1:M:220:ILE:HG13	2.17	0.44
1:M:449:ALA:N	1:M:450:PRO:CD	2.81	0.44
1:M:524:LEU:HG	1:M:525:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:242:LYS:O	1:T:243:ALA:CB	2.64	0.44
1:a:16:MET:HB3	1:a:514:MET:HE3	1.99	0.44
1:A:217:SER:N	1:A:218:PRO:HD3	2.33	0.43
2:D:17:LEU:HA	2:D:20:VAL:HG12	2.00	0.43
2:E:292:ILE:O	2:E:296:THR:HG22	2.17	0.43
1:F:14:VAL:O	1:F:18:ARG:HG3	2.18	0.43
1:G:230:ILE:N	1:G:257:GLU:OE1	2.51	0.43
2:K:5:ASP:HB2	2:K:524:LEU:HD12	2.00	0.43
2:K:355:GLU:HB3	6:K:704:HOH:O	2.18	0.43
1:N:220:ILE:HD12	1:N:319:GLN:HA	2.00	0.43
2:R:17:LEU:HA	2:R:20:VAL:HG22	2.00	0.43
2:R:220:ILE:HD11	2:R:250:ILE:CD1	2.48	0.43
2:W:5:ASP:HB2	2:W:524:LEU:HD23	1.99	0.43
2:W:449:ALA:HB3	2:W:450:PRO:HD3	1.99	0.43
1:A:165:ALA:HA	1:A:187:LEU:HD11	2.00	0.43
2:K:88:GLY:CA	2:K:91:THR:HG22	2.48	0.43
2:K:417:VAL:HG21	2:K:488:MET:HG3	1.99	0.43
1:M:217:SER:N	1:M:218:PRO:HD3	2.32	0.43
2:O:17:LEU:HA	2:O:20:VAL:HG22	2.00	0.43
2:V:353:ILE:HG23	2:V:362:ARG:HG2	2.00	0.43
2:V:449:ALA:HB3	2:V:450:PRO:HD3	1.99	0.43
2:c:16:MET:HB3	2:c:514:MET:HE3	1.99	0.43
1:A:213:VAL:HG12	1:A:215:LEU:CD1	2.47	0.43
2:D:220:ILE:HG22	2:D:318:GLY:C	2.44	0.43
1:F:193:MET:HG3	1:F:371:LYS:HB3	2.00	0.43
1:H:217:SER:N	1:H:218:PRO:HD3	2.33	0.43
2:Z:77:VAL:HG11	2:Z:510:VAL:HG13	2.01	0.43
2:Z:261:THR:HA	2:Z:264:VAL:HG22	2.00	0.43
1:b:203:TYR:HB2	1:b:263:VAL:CG2	2.49	0.43
1:B:200:LEU:HD21	1:B:277:LYS:HG3	2.00	0.43
1:P:514:MET:HE3	1:P:514:MET:HB2	1.92	0.43
1:b:193:MET:HG3	1:b:371:LYS:HB3	2.00	0.43
1:b:449:ALA:HB3	1:b:450:PRO:HD3	1.99	0.43
1:C:266:THR:CG2	1:C:273:VAL:HG12	2.48	0.43
2:E:336:VAL:O	2:E:336:VAL:HG12	2.18	0.43
1:F:248:LEU:HD13	1:F:325:ILE:HD11	2.01	0.43
1:N:449:ALA:HB3	1:N:450:PRO:HD3	2.00	0.43
2:R:248:LEU:HD13	2:R:325:ILE:HD11	2.00	0.43
1:U:353:ILE:HG23	1:U:362:ARG:HG2	2.00	0.43
2:V:146:GLN:O	2:V:149:THR:HG22	2.17	0.43
2:V:200:LEU:HD21	2:V:277:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:215:LEU:HB2	2:Z:323:VAL:HG22	2.00	0.43
2:c:17:LEU:HA	2:c:20:VAL:HG22	2.01	0.43
1:F:233:MET:SD	1:F:262:LEU:HD11	2.58	0.43
1:G:248:LEU:HD13	1:G:325:ILE:HD11	1.99	0.43
1:Q:248:LEU:HD13	1:Q:325:ILE:HD11	2.01	0.43
2:V:296:THR:HG23	2:V:318:GLY:HA3	2.01	0.43
2:V:449:ALA:N	2:V:450:PRO:CD	2.81	0.43
2:X:193:MET:HG3	2:X:371:LYS:HB3	1.99	0.43
1:b:193:MET:HB2	1:b:295:LEU:HD22	2.01	0.43
1:B:210:THR:HG23	1:B:212:ALA:HB3	2.01	0.43
1:C:449:ALA:HB3	1:C:450:PRO:HD3	2.01	0.43
2:D:217:SER:N	2:D:218:PRO:HD3	2.33	0.43
2:D:501:ARG:HH12	4:D:604:HEZ:H11	1.84	0.43
1:G:305:ILE:HG22	1:G:305:ILE:O	2.19	0.43
1:H:69:MET:HE2	1:N:39:VAL:HG12	2.00	0.43
1:P:449:ALA:HB3	1:P:450:PRO:HD3	2.01	0.43
2:W:180:GLY:HA2	2:W:380:LYS:HB3	2.00	0.43
2:W:248:LEU:HD13	2:W:325:ILE:HD11	2.01	0.43
1:Y:223:ALA:HA	1:Y:301:ILE:HG22	1.99	0.43
1:a:36:ARG:HD3	1:b:114:MET:HE2	2.00	0.43
2:D:193:MET:HG3	2:D:371:LYS:HB3	2.00	0.43
2:D:242:LYS:O	2:D:243:ALA:CB	2.66	0.43
1:F:49:ILE:HD11	1:G:73:MET:HE3	2.00	0.43
2:K:222:LEU:HD11	2:K:293:ALA:HA	2.00	0.43
1:M:302:SER:HB3	1:M:304:GLU:HG2	1.99	0.43
1:Q:186:GLU:HB2	1:Q:380:LYS:HB2	2.00	0.43
1:Q:501:ARG:HH12	4:Q:604:HEZ:H22	1.84	0.43
2:R:77:VAL:HG11	2:R:510:VAL:HG13	2.01	0.43
1:T:449:ALA:HB3	1:T:450:PRO:HD3	2.00	0.43
2:Z:449:ALA:HB3	2:Z:450:PRO:HD3	1.99	0.43
2:E:193:MET:HG3	2:E:371:LYS:HB3	2.01	0.43
1:I:449:ALA:HB3	1:I:450:PRO:HD3	2.01	0.43
1:M:17:LEU:HA	1:M:20:VAL:HG22	2.00	0.43
2:R:305:ILE:O	2:R:305:ILE:HG22	2.17	0.43
1:a:250:ILE:HD13	1:a:276:VAL:HG22	2.01	0.43
1:A:301:ILE:HG21	1:A:309:LEU:HD12	2.00	0.43
1:F:220:ILE:C	1:F:220:ILE:HD12	2.44	0.43
2:V:266:THR:HG23	2:V:273:VAL:HG12	2.01	0.43
2:c:191:GLU:OE2	3:c:601:BME:H22	2.19	0.43
1:A:269:GLY:O	1:B:229:ASN:ND2	2.52	0.42
1:C:176:THR:HG21	1:C:333:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:262:LEU:HD22	1:Q:273:VAL:HG11	2.01	0.42
2:R:186:GLU:HB2	2:R:380:LYS:HB2	2.01	0.42
1:U:17:LEU:HA	1:U:20:VAL:HG22	2.00	0.42
2:V:5:ASP:HB2	2:V:524:LEU:HD23	2.01	0.42
2:Z:443:ALA:O	2:Z:447:MET:HG3	2.19	0.42
1:a:291:ASP:HB3	1:a:372:LEU:HD11	2.01	0.42
1:A:524:LEU:HD12	1:A:524:LEU:HA	1.93	0.42
1:C:449:ALA:N	1:C:450:PRO:CD	2.81	0.42
2:E:233:MET:HA	2:E:233:MET:CE	2.44	0.42
1:M:302:SER:H	1:M:307:MET:HE3	1.84	0.42
2:X:227:ILE:HD11	2:X:254:VAL:HG22	2.01	0.42
1:B:314:LEU:HD12	1:B:314:LEU:HA	1.93	0.42
1:G:314:LEU:C	1:G:314:LEU:HD12	2.44	0.42
2:K:305:ILE:O	2:K:305:ILE:CG2	2.67	0.42
2:L:222:LEU:HD23	2:L:250:ILE:CG1	2.49	0.42
2:L:227:ILE:HD11	2:L:254:VAL:HG22	1.99	0.42
2:V:385:THR:HG22	2:V:387:VAL:H	1.84	0.42
2:X:205:ILE:CD1	2:X:211:GLY:HA2	2.45	0.42
1:G:254:VAL:HG11	1:G:275:ALA:HB1	2.01	0.42
1:H:193:MET:HG3	1:H:371:LYS:HB3	2.01	0.42
2:L:301:ILE:O	2:L:301:ILE:CG2	2.67	0.42
1:Q:230:ILE:HD12	1:Q:230:ILE:C	2.45	0.42
2:R:305:ILE:O	2:R:305:ILE:CG2	2.66	0.42
2:W:146:GLN:O	2:W:149:THR:HG22	2.19	0.42
2:W:166:MET:HE2	2:W:171:LYS:HA	2.01	0.42
2:Z:77:VAL:HG21	2:Z:510:VAL:HG13	1.99	0.42
2:c:449:ALA:N	2:c:450:PRO:CD	2.82	0.42
2:K:29:VAL:HG12	3:K:601:BME:C1	2.49	0.42
1:Q:77:VAL:HG11	1:Q:510:VAL:HG13	2.02	0.42
2:R:77:VAL:HG21	2:R:510:VAL:HG13	2.01	0.42
2:R:210:THR:HG23	2:R:212:ALA:HB3	2.00	0.42
2:R:220:ILE:HG22	2:R:318:GLY:C	2.44	0.42
2:R:324:VAL:CG2	2:R:331:THR:CG2	2.96	0.42
2:V:248:LEU:HD13	2:V:325:ILE:HD11	2.02	0.42
2:W:305:ILE:O	2:W:305:ILE:HG22	2.19	0.42
2:Z:77:VAL:CG2	2:Z:510:VAL:CG1	2.95	0.42
1:F:169:VAL:HG12	1:F:169:VAL:O	2.19	0.42
1:I:319:GLN:HG3	1:I:336:VAL:HG21	2.00	0.42
2:K:220:ILE:CD1	2:K:296:THR:HG21	2.46	0.42
2:O:200:LEU:HD21	2:O:277:LYS:HG3	2.02	0.42
1:Y:246:PRO:HB3	1:Y:272:LYS:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:387:VAL:O	1:Y:391:GLU:HG2	2.20	0.42
1:a:417:VAL:HG21	1:a:488:MET:HG3	2.01	0.42
1:A:305:ILE:CG1	1:A:307:MET:HE2	2.50	0.42
1:C:210:THR:HG23	1:C:212:ALA:HB3	2.02	0.42
1:C:223:ALA:HA	1:C:301:ILE:HG22	2.01	0.42
2:E:17:LEU:HA	2:E:20:VAL:HG12	2.01	0.42
1:F:220:ILE:HD12	1:F:220:ILE:O	2.19	0.42
1:F:234:LEU:N	1:F:235:PRO:CD	2.81	0.42
1:I:200:LEU:HD21	1:I:277:LYS:HG3	2.01	0.42
2:O:114:MET:CE	1:U:36:ARG:HD3	2.48	0.42
1:Q:449:ALA:N	1:Q:450:PRO:CD	2.82	0.42
1:U:248:LEU:HD13	1:U:325:ILE:HD11	2.00	0.42
2:V:227:ILE:HD11	2:V:254:VAL:HG22	2.01	0.42
1:Y:217:SER:N	1:Y:218:PRO:HD3	2.35	0.42
2:E:514:MET:HE2	2:E:514:MET:HB3	1.92	0.42
1:G:223:ALA:HA	1:G:301:ILE:HG22	2.01	0.42
1:G:314:LEU:HA	1:G:317:LEU:HD12	2.01	0.42
1:J:291:ASP:HB3	1:J:372:LEU:HD11	2.01	0.42
1:M:230:ILE:O	1:M:234:LEU:HD13	2.20	0.42
2:O:248:LEU:HD13	2:O:325:ILE:HD11	2.00	0.42
1:Q:291:ASP:HB3	1:Q:372:LEU:HD11	2.02	0.42
1:T:259:LEU:C	1:T:259:LEU:HD23	2.45	0.42
2:W:319:GLN:HG3	2:W:336:VAL:HG21	2.02	0.42
2:X:183:LEU:C	2:X:183:LEU:HD13	2.45	0.42
2:X:200:LEU:HD11	2:X:277:LYS:HG3	2.02	0.42
2:Z:186:GLU:HB2	2:Z:380:LYS:HB2	2.01	0.42
1:a:308:GLU:HB2	1:a:311:LYS:HE3	2.01	0.42
1:b:16:MET:HB3	1:b:514:MET:HE3	2.00	0.42
2:c:449:ALA:HB3	2:c:450:PRO:HD3	2.01	0.42
1:F:230:ILE:HA	1:F:233:MET:HG2	2.02	0.42
1:H:248:LEU:HD13	1:H:325:ILE:HD11	2.00	0.42
1:H:271:VAL:HG12	1:H:273:VAL:HG23	2.02	0.42
2:L:443:ALA:O	2:L:447:MET:HG3	2.20	0.42
1:P:353:ILE:HG23	1:P:362:ARG:HG2	2.02	0.42
1:Y:183:LEU:HD13	1:Y:183:LEU:O	2.20	0.42
2:Z:200:LEU:HD21	2:Z:277:LYS:HG3	2.02	0.42
2:Z:345:ARG:HH21	2:Z:368:ARG:HH22	1.67	0.42
1:a:222:LEU:O	1:a:301:ILE:HG22	2.20	0.42
1:G:449:ALA:N	1:G:450:PRO:CD	2.83	0.42
2:K:346:VAL:HG13	2:K:369:VAL:HG23	2.01	0.42
2:L:166:MET:HE2	2:L:171:LYS:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:449:ALA:N	1:P:450:PRO:CD	2.83	0.42
1:T:524:LEU:HG	1:T:525:PRO:HD2	2.02	0.42
1:U:217:SER:N	1:U:218:PRO:HD3	2.35	0.42
2:W:250:ILE:HD13	2:W:276:VAL:HG22	2.02	0.42
1:a:230:ILE:CG2	1:a:261:THR:OG1	2.67	0.42
2:c:43:SER:OG	2:c:44:PHE:N	2.53	0.42
1:A:200:LEU:HD21	1:A:277:LYS:HG3	2.02	0.41
1:C:301:ILE:O	1:C:301:ILE:CG2	2.67	0.41
2:D:305:ILE:O	2:D:305:ILE:CG2	2.68	0.41
1:G:220:ILE:HD12	1:G:296:THR:CG2	2.50	0.41
2:K:186:GLU:HB2	2:K:380:LYS:HB2	2.02	0.41
2:K:230:ILE:HG13	2:K:261:THR:OG1	2.20	0.41
2:R:313:THR:OG1	2:R:314:LEU:N	2.53	0.41
2:X:291:ASP:HB3	2:X:372:LEU:HD11	2.01	0.41
1:Y:239:ALA:HB1	1:Y:314:LEU:HG	2.02	0.41
2:Z:77:VAL:HG21	2:Z:510:VAL:HG12	2.02	0.41
2:c:77:VAL:HG21	2:c:510:VAL:HG12	2.02	0.41
1:G:222:LEU:HD23	1:G:250:ILE:CG1	2.51	0.41
1:I:16:MET:HB3	1:I:514:MET:HE3	2.02	0.41
2:K:250:ILE:CD1	2:K:276:VAL:HG13	2.50	0.41
2:O:443:ALA:O	2:O:447:MET:HG3	2.20	0.41
1:Q:385:THR:CG2	1:Q:387:VAL:HG12	2.51	0.41
2:R:16:MET:HB3	2:R:514:MET:HE3	2.02	0.41
2:W:443:ALA:O	2:W:447:MET:HG3	2.20	0.41
2:c:77:VAL:CG2	2:c:510:VAL:CG1	2.98	0.41
1:C:291:ASP:HB3	1:C:372:LEU:HD11	2.03	0.41
2:D:353:ILE:HG23	2:D:362:ARG:HG2	2.03	0.41
1:F:217:SER:N	1:F:218:PRO:HD3	2.35	0.41
1:G:353:ILE:HG23	1:G:362:ARG:HG2	2.01	0.41
1:J:449:ALA:N	1:J:450:PRO:CD	2.83	0.41
2:K:222:LEU:CD1	2:K:293:ALA:HB2	2.50	0.41
2:L:301:ILE:HD11	2:L:308:GLU:O	2.20	0.41
1:M:169:VAL:HG12	1:M:173:GLY:HA3	2.02	0.41
2:O:220:ILE:HD12	2:O:319:GLN:HA	2.01	0.41
2:R:248:LEU:HD22	2:R:323:VAL:HG11	2.02	0.41
1:T:200:LEU:HD21	1:T:277:LYS:HG3	2.02	0.41
2:W:449:ALA:N	2:W:450:PRO:CD	2.83	0.41
2:X:249:ILE:HD11	2:X:275:ALA:HB2	2.02	0.41
1:C:203:TYR:HB3	1:C:267:MET:HE2	2.03	0.41
1:F:220:ILE:CD1	1:F:222:LEU:HG	2.50	0.41
1:F:259:LEU:C	1:F:259:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:223:ALA:O	2:O:251:ALA:HA	2.21	0.41
2:W:389:MET:HG3	2:W:390:LYS:N	2.34	0.41
1:b:217:SER:N	1:b:218:PRO:HD3	2.35	0.41
1:G:222:LEU:HD22	1:G:250:ILE:HD11	1.98	0.41
1:H:39:VAL:HG12	1:I:69:MET:HE2	2.03	0.41
1:I:248:LEU:HD13	1:I:325:ILE:HD11	2.01	0.41
1:I:514:MET:HE2	1:I:514:MET:HB3	1.89	0.41
2:K:233:MET:HE1	2:K:262:LEU:HD11	2.01	0.41
2:K:353:ILE:HD11	2:K:365:LEU:CB	2.51	0.41
1:Y:311:LYS:O	1:Y:311:LYS:HG2	2.20	0.41
2:c:514:MET:HE2	2:c:514:MET:HB3	1.88	0.41
1:H:319:GLN:HG3	1:H:336:VAL:HG21	2.01	0.41
1:M:346:VAL:HG13	1:M:369:VAL:HG23	2.02	0.41
1:Q:202:PRO:O	1:Q:205:ILE:HG12	2.19	0.41
2:R:114:MET:HB3	2:R:118:ARG:HH12	1.85	0.41
1:Y:301:ILE:O	1:Y:301:ILE:CG2	2.67	0.41
2:Z:198:GLY:O	2:Z:276:VAL:HG23	2.20	0.41
1:a:59:GLU:O	1:b:4:LYS:NZ	2.53	0.41
1:G:203:TYR:CD2	1:G:267:MET:HE3	2.56	0.41
1:U:514:MET:HE2	1:U:514:MET:HB3	1.93	0.41
1:Y:348:GLN:O	1:Y:351:GLN:HB3	2.21	0.41
2:c:291:ASP:HB3	2:c:372:LEU:HD11	2.03	0.41
1:B:417:VAL:HG21	1:B:488:MET:HG3	2.02	0.41
1:N:443:ALA:O	1:N:447:MET:HG3	2.20	0.41
2:O:193:MET:HG3	2:O:371:LYS:HB3	2.02	0.41
1:U:230:ILE:C	1:U:230:ILE:HD12	2.45	0.41
2:W:230:ILE:HG13	2:W:261:THR:HB	2.02	0.41
2:W:234:LEU:N	2:W:235:PRO:CD	2.83	0.41
2:X:5:ASP:HB2	2:X:524:LEU:HD23	2.02	0.41
2:Z:17:LEU:HA	2:Z:20:VAL:HG22	2.03	0.41
1:A:233:MET:HE1	1:A:249:ILE:HD13	2.03	0.41
1:A:302:SER:H	1:A:307:MET:HE3	1.86	0.41
1:C:227:ILE:HD11	1:C:309:LEU:HD11	2.02	0.41
1:C:248:LEU:HD13	1:C:325:ILE:HD11	2.02	0.41
1:C:262:LEU:HG	1:C:273:VAL:HG11	2.02	0.41
1:H:443:ALA:O	1:H:447:MET:HG3	2.20	0.41
2:K:449:ALA:N	2:K:450:PRO:CD	2.84	0.41
2:L:223:ALA:O	2:L:251:ALA:HA	2.20	0.41
1:N:193:MET:HG3	1:N:371:LYS:HB3	2.02	0.41
1:Q:346:VAL:HG13	1:Q:369:VAL:HG23	2.02	0.41
1:Q:449:ALA:HB3	1:Q:450:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:514:MET:HE2	2:R:514:MET:HB3	1.89	0.41
2:W:305:ILE:O	2:W:305:ILE:CG2	2.68	0.41
2:X:230:ILE:O	2:X:233:MET:HG2	2.21	0.41
2:X:420:ILE:HG13	2:X:448:GLU:HG2	2.03	0.41
1:Y:203:TYR:HB3	1:Y:267:MET:HE2	2.02	0.41
1:a:301:ILE:HG21	1:a:309:LEU:CD1	2.51	0.41
1:b:353:ILE:HG23	1:b:362:ARG:HG2	2.03	0.41
2:c:217:SER:N	2:c:218:PRO:HD3	2.36	0.41
1:A:186:GLU:HB2	1:A:380:LYS:HB2	2.02	0.41
1:A:266:THR:HG22	1:A:273:VAL:H	1.85	0.41
2:K:225:LYS:HD2	2:K:309:LEU:HD13	2.03	0.41
2:K:278:ALA:HB1	2:K:289:LEU:CD2	2.44	0.41
2:L:77:VAL:HG11	2:L:510:VAL:HG13	2.03	0.41
2:O:346:VAL:HG13	2:O:369:VAL:HG23	2.02	0.41
1:Q:210:THR:HG23	1:Q:212:ALA:HB3	2.03	0.41
1:U:443:ALA:O	1:U:447:MET:HG3	2.21	0.41
2:W:220:ILE:HD12	2:W:296:THR:CG2	2.51	0.41
1:B:525:PRO:O	1:B:526:LYS:C	2.64	0.40
2:E:49:ILE:CD1	1:F:73:MET:HE3	2.52	0.40
2:E:77:VAL:CG2	2:E:510:VAL:CG1	2.98	0.40
2:E:220:ILE:CD1	2:E:332:ILE:HD11	2.51	0.40
1:G:204:PHE:CE1	1:G:263:VAL:HG22	2.56	0.40
1:G:250:ILE:HG22	1:G:276:VAL:HG22	2.00	0.40
1:M:443:ALA:O	1:M:447:MET:HG3	2.21	0.40
2:O:5:ASP:HB2	2:O:524:LEU:HD23	2.02	0.40
1:P:417:VAL:HG21	1:P:488:MET:HG3	2.02	0.40
1:Y:260:ALA:O	1:Y:263:VAL:HG12	2.21	0.40
1:A:234:LEU:N	1:A:235:PRO:CD	2.84	0.40
1:C:266:THR:HG22	1:C:273:VAL:H	1.86	0.40
1:H:77:VAL:HG11	1:H:510:VAL:HG13	2.03	0.40
2:R:217:SER:N	2:R:218:PRO:HD3	2.36	0.40
2:R:449:ALA:N	2:R:450:PRO:CD	2.84	0.40
2:W:193:MET:HG3	2:W:371:LYS:HB3	2.04	0.40
1:Y:44:PHE:O	1:Y:44:PHE:CD2	2.75	0.40
2:Z:5:ASP:HB2	2:Z:524:LEU:HD12	2.02	0.40
2:D:166:MET:HE2	2:D:171:LYS:HA	2.03	0.40
2:L:17:LEU:HA	2:L:20:VAL:HG22	2.03	0.40
4:R:604:HEZ:H61	4:R:604:HEZ:H31	1.76	0.40
1:U:104:LEU:HA	1:U:107:VAL:HG22	2.03	0.40
1:B:227:ILE:HD11	1:B:309:LEU:HD11	2.02	0.40
1:B:524:LEU:HD12	1:B:524:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:VAL:HG12	1:C:173:GLY:HA3	2.04	0.40
2:D:5:ASP:HB2	2:D:524:LEU:HD23	2.04	0.40
1:J:271:VAL:HG12	1:J:273:VAL:HG23	2.04	0.40
2:L:301:ILE:HG21	2:L:309:LEU:CD1	2.51	0.40
1:N:506:TYR:CE1	4:N:602:HEZ:H62	2.57	0.40
2:O:217:SER:N	2:O:218:PRO:HD3	2.37	0.40
2:R:4:LYS:HE2	6:R:704:HOH:O	2.19	0.40
2:V:193:MET:HB2	2:V:295:LEU:HD22	2.04	0.40
2:Z:291:ASP:HB3	2:Z:372:LEU:HD11	2.04	0.40
1:a:213:VAL:HG13	1:a:325:ILE:HB	1.99	0.40
1:a:443:ALA:O	1:a:447:MET:HG3	2.22	0.40
1:B:449:ALA:N	1:B:450:PRO:CD	2.84	0.40
1:C:169:VAL:HG12	1:C:169:VAL:O	2.21	0.40
1:F:73:MET:HE2	1:F:514:MET:HE2	2.03	0.40
1:G:22:VAL:HG11	1:G:62:LEU:HD21	2.04	0.40
2:L:222:LEU:HD13	2:L:293:ALA:HB2	2.02	0.40
2:L:449:ALA:HB3	2:L:450:PRO:HD3	2.04	0.40
2:O:77:VAL:CG2	2:O:510:VAL:CG1	2.97	0.40
1:U:501:ARG:HH12	4:U:604:HEZ:C1	2.34	0.40

There are no symmetry-related clashes.

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	522/548 (95%)	511 (98%)	11 (2%)	0	100	100
1	B	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	C	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	F	521/548 (95%)	513 (98%)	8 (2%)	0	100	100
1	G	522/548 (95%)	514 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	I	521/548 (95%)	514 (99%)	7 (1%)	0	100	100
1	J	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	M	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	N	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	P	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
1	Q	522/548 (95%)	516 (99%)	6 (1%)	0	100	100
1	T	522/548 (95%)	515 (99%)	7 (1%)	0	100	100
1	U	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	Y	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
1	a	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
1	b	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
2	D	523/548 (95%)	514 (98%)	9 (2%)	0	100	100
2	E	523/548 (95%)	513 (98%)	10 (2%)	0	100	100
2	K	523/548 (95%)	516 (99%)	7 (1%)	0	100	100
2	L	523/548 (95%)	515 (98%)	8 (2%)	0	100	100
2	O	523/548 (95%)	516 (99%)	7 (1%)	0	100	100
2	R	523/548 (95%)	515 (98%)	8 (2%)	0	100	100
2	V	523/548 (95%)	515 (98%)	8 (2%)	0	100	100
2	W	523/548 (95%)	515 (98%)	8 (2%)	0	100	100
2	X	523/548 (95%)	514 (98%)	9 (2%)	0	100	100
2	Z	523/548 (95%)	512 (98%)	11 (2%)	0	100	100
2	c	523/548 (95%)	515 (98%)	8 (2%)	0	100	100
All	All	14625/15344 (95%)	14415 (99%)	210 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	404/414 (98%)	403 (100%)	1 (0%)	92	97
1	B	404/414 (98%)	402 (100%)	2 (0%)	86	94
1	C	404/414 (98%)	401 (99%)	3 (1%)	81	91
1	F	403/414 (97%)	403 (100%)	0	100	100
1	G	404/414 (98%)	403 (100%)	1 (0%)	92	97
1	H	404/414 (98%)	404 (100%)	0	100	100
1	I	403/414 (97%)	401 (100%)	2 (0%)	86	94
1	J	404/414 (98%)	402 (100%)	2 (0%)	86	94
1	M	404/414 (98%)	402 (100%)	2 (0%)	86	94
1	N	404/414 (98%)	402 (100%)	2 (0%)	86	94
1	P	404/414 (98%)	404 (100%)	0	100	100
1	Q	404/414 (98%)	402 (100%)	2 (0%)	86	94
1	T	404/414 (98%)	402 (100%)	2 (0%)	86	94
1	U	404/414 (98%)	404 (100%)	0	100	100
1	Y	404/414 (98%)	403 (100%)	1 (0%)	92	97
1	a	404/414 (98%)	403 (100%)	1 (0%)	92	97
1	b	404/414 (98%)	403 (100%)	1 (0%)	92	97
2	D	405/415 (98%)	404 (100%)	1 (0%)	92	97
2	E	405/415 (98%)	403 (100%)	2 (0%)	86	94
2	K	405/415 (98%)	405 (100%)	0	100	100
2	L	405/415 (98%)	402 (99%)	3 (1%)	81	91
2	O	405/415 (98%)	405 (100%)	0	100	100
2	R	405/415 (98%)	402 (99%)	3 (1%)	81	91
2	V	405/415 (98%)	405 (100%)	0	100	100
2	W	405/415 (98%)	405 (100%)	0	100	100
2	X	405/415 (98%)	404 (100%)	1 (0%)	92	97
2	Z	405/415 (98%)	404 (100%)	1 (0%)	92	97
2	c	405/415 (98%)	405 (100%)	0	100	100
All	All	11321/11603 (98%)	11288 (100%)	33 (0%)	91	96

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	493	ILE
1	B	230	ILE
1	B	315	GLU
1	C	236	VAL
1	C	333	ILE
1	C	362	ARG
2	D	82	ASN
2	E	213	VAL
2	E	245	LYS
1	G	245	LYS
1	I	82	ASN
1	I	359	ASP
1	J	172	GLU
1	J	359	ASP
2	L	213	VAL
2	L	422	VAL
2	L	526	LYS
1	M	82	ASN
1	M	313	THR
1	N	268	ARG
1	N	321	LYS
1	Q	156	GLU
1	Q	304	GLU
2	R	82	ASN
2	R	313	THR
2	R	359	ASP
1	T	295	LEU
1	T	359	ASP
2	X	82	ASN
1	Y	352	GLN
2	Z	422	VAL
1	a	207	LYS
1	b	160	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	97	GLN
1	A	290	GLN
1	A	453	GLN
1	A	475	ASN
1	B	10	ASN

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Mol	Chain	Res	Type
1	B	72	GLN
1	B	97	GLN
1	B	366	GLN
1	B	453	GLN
1	C	72	GLN
1	C	97	GLN
1	C	194	GLN
1	C	265	ASN
1	C	343	GLN
1	C	453	GLN
1	C	475	ASN
1	C	479	ASN
2	D	97	GLN
2	D	184	GLN
2	D	229	ASN
2	D	265	ASN
2	D	343	GLN
2	D	475	ASN
2	D	479	ASN
2	E	343	GLN
2	E	453	GLN
2	E	475	ASN
2	E	479	ASN
1	F	97	GLN
1	F	112	ASN
1	F	453	GLN
1	F	475	ASN
1	G	343	GLN
1	G	352	GLN
1	G	366	GLN
1	G	453	GLN
1	G	475	ASN
1	G	479	ASN
1	H	97	GLN
1	H	194	GLN
1	H	366	GLN
1	H	453	GLN
1	H	475	ASN
1	I	453	GLN
1	I	475	ASN
1	I	479	ASN
1	J	348	GLN

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Mol	Chain	Res	Type
1	J	366	GLN
1	J	453	GLN
1	J	475	ASN
2	K	194	GLN
2	K	290	GLN
2	K	351	GLN
2	K	453	GLN
2	K	475	ASN
2	L	97	GLN
2	L	194	GLN
2	L	453	GLN
2	L	475	ASN
2	L	479	ASN
1	M	97	GLN
1	M	229	ASN
1	M	475	ASN
1	M	479	ASN
1	N	21	ASN
1	N	97	GLN
1	N	453	GLN
1	N	475	ASN
2	O	72	GLN
2	O	97	GLN
2	O	194	GLN
2	O	401	HIS
2	O	453	GLN
2	O	475	ASN
2	O	479	ASN
1	P	37	ASN
1	P	184	GLN
1	P	366	GLN
1	P	475	ASN
1	Q	68	ASN
1	Q	97	GLN
1	Q	475	ASN
1	Q	479	ASN
2	R	37	ASN
2	R	72	GLN
2	R	97	GLN
2	R	290	GLN
2	R	343	GLN
2	R	453	GLN

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Mol	Chain	Res	Type
2	R	475	ASN
2	R	479	ASN
1	T	97	GLN
1	T	453	GLN
1	T	475	ASN
1	T	479	ASN
1	U	72	GLN
1	U	97	GLN
1	U	194	GLN
1	U	453	GLN
1	U	475	ASN
1	U	479	ASN
2	V	72	GLN
2	V	229	ASN
2	V	453	GLN
2	V	475	ASN
2	V	479	ASN
2	W	97	GLN
2	W	290	GLN
2	W	453	GLN
2	W	475	ASN
2	W	479	ASN
2	X	194	GLN
2	X	453	GLN
2	X	475	ASN
2	X	479	ASN
1	Y	97	GLN
1	Y	229	ASN
1	Y	265	ASN
1	Y	348	GLN
1	Y	453	GLN
2	Z	112	ASN
2	Z	366	GLN
2	Z	453	GLN
1	a	97	GLN
1	a	453	GLN
1	a	475	ASN
1	b	97	GLN
1	b	194	GLN
1	b	229	ASN
1	b	453	GLN
1	b	475	ASN

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Mol	Chain	Res	Type
2	c	37	ASN
2	c	97	GLN
2	c	453	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

17 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	B	43	1	8,9,10	0.69	0	8,12,14	0.58	0
1	SEP	A	43	1	8,9,10	0.78	0	8,12,14	0.54	0
1	SEP	F	43	1	8,9,10	0.66	0	8,12,14	0.59	0
1	SEP	N	43	1	8,9,10	0.78	0	8,12,14	0.59	0
1	SEP	G	43	1	8,9,10	0.74	0	8,12,14	0.60	0
1	SEP	J	43	1	8,9,10	0.77	0	8,12,14	0.56	0
1	SEP	M	43	1	8,9,10	0.74	0	8,12,14	0.59	0
1	SEP	H	43	1	8,9,10	0.74	0	8,12,14	0.59	0
1	SEP	Q	43	1	8,9,10	0.74	0	8,12,14	0.57	0
1	SEP	T	43	1	8,9,10	0.78	0	8,12,14	0.54	0
1	SEP	U	43	1	8,9,10	0.77	0	8,12,14	0.57	0
1	SEP	Y	43	1	8,9,10	0.64	0	8,12,14	0.58	0
1	SEP	a	43	1	8,9,10	0.71	0	8,12,14	0.60	0
1	SEP	C	43	1	8,9,10	0.81	0	8,12,14	0.62	0
1	SEP	b	43	1	8,9,10	0.62	0	8,12,14	0.60	0
1	SEP	I	43	1	8,9,10	0.79	0	8,12,14	0.54	0
1	SEP	P	43	1	8,9,10	0.68	0	8,12,14	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	43	1	-	1/5/8/10	-
1	SEP	A	43	1	-	3/5/8/10	-
1	SEP	F	43	1	-	2/5/8/10	-
1	SEP	N	43	1	-	2/5/8/10	-
1	SEP	G	43	1	-	3/5/8/10	-
1	SEP	J	43	1	-	3/5/8/10	-
1	SEP	M	43	1	-	4/5/8/10	-
1	SEP	H	43	1	-	2/5/8/10	-
1	SEP	Q	43	1	-	2/5/8/10	-
1	SEP	T	43	1	-	3/5/8/10	-
1	SEP	U	43	1	-	3/5/8/10	-
1	SEP	Y	43	1	-	3/5/8/10	-
1	SEP	a	43	1	-	2/5/8/10	-
1	SEP	C	43	1	-	4/5/8/10	-
1	SEP	b	43	1	-	1/5/8/10	-
1	SEP	I	43	1	-	2/5/8/10	-
1	SEP	P	43	1	-	2/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	43	SEP	N-CA-CB-OG
1	A	43	SEP	CA-CB-OG-P
1	C	43	SEP	CB-OG-P-O2P
1	C	43	SEP	CB-OG-P-O3P
1	F	43	SEP	CA-CB-OG-P
1	G	43	SEP	CA-CB-OG-P
1	H	43	SEP	CA-CB-OG-P
1	I	43	SEP	CA-CB-OG-P
1	J	43	SEP	CA-CB-OG-P
1	M	43	SEP	N-CA-CB-OG
1	M	43	SEP	CA-CB-OG-P
1	M	43	SEP	CB-OG-P-O1P

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Mol	Chain	Res	Type	Atoms
1	N	43	SEP	CA-CB-OG-P
1	P	43	SEP	N-CA-CB-OG
1	P	43	SEP	CA-CB-OG-P
1	Q	43	SEP	CA-CB-OG-P
1	T	43	SEP	CA-CB-OG-P
1	U	43	SEP	CA-CB-OG-P
1	Y	43	SEP	N-CA-CB-OG
1	Y	43	SEP	CA-CB-OG-P
1	a	43	SEP	CA-CB-OG-P
1	b	43	SEP	CA-CB-OG-P
1	G	43	SEP	CB-OG-P-O1P
1	J	43	SEP	CB-OG-P-O1P
1	U	43	SEP	CB-OG-P-O1P
1	B	43	SEP	CA-CB-OG-P
1	C	43	SEP	CA-CB-OG-P
1	C	43	SEP	N-CA-CB-OG
1	F	43	SEP	N-CA-CB-OG
1	H	43	SEP	N-CA-CB-OG
1	I	43	SEP	N-CA-CB-OG
1	J	43	SEP	N-CA-CB-OG
1	N	43	SEP	N-CA-CB-OG
1	Q	43	SEP	N-CA-CB-OG
1	T	43	SEP	N-CA-CB-OG
1	a	43	SEP	N-CA-CB-OG
1	A	43	SEP	CB-OG-P-O1P
1	T	43	SEP	CB-OG-P-O1P
1	Y	43	SEP	CB-OG-P-O1P
1	G	43	SEP	CB-OG-P-O3P
1	M	43	SEP	CB-OG-P-O2P
1	U	43	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	43	SEP	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 100 ligands modelled in this entry, 14 are monoatomic - leaving 86 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	HEZ	E	605	-	7,7,7	0.07	0	6,6,6	0.14	0
3	BME	F	601	-	3,3,3	0.21	0	1,2,2	0.25	0
4	HEZ	F	603	-	7,7,7	0.20	0	6,6,6	0.13	0
4	HEZ	W	602	-	7,7,7	0.18	0	6,6,6	0.08	0
3	BME	A	601	-	3,3,3	0.18	0	1,2,2	0.30	0
4	HEZ	H	602	-	7,7,7	0.08	0	6,6,6	0.13	0
4	HEZ	N	602	-	7,7,7	0.20	0	6,6,6	0.14	0
4	HEZ	Q	604	-	7,7,7	0.23	0	6,6,6	0.12	0
4	HEZ	c	605	-	7,7,7	0.11	0	6,6,6	0.12	0
4	HEZ	O	605	-	7,7,7	0.13	0	6,6,6	0.12	0
4	HEZ	O	604	-	7,7,7	0.13	0	6,6,6	0.11	0
3	BME	U	602	-	3,3,3	0.20	0	1,2,2	0.10	0
4	HEZ	U	604	-	7,7,7	0.20	0	6,6,6	0.13	0
3	BME	U	603	-	3,3,3	0.15	0	1,2,2	0.01	0
3	BME	R	601	-	3,3,3	0.22	0	1,2,2	0.21	0
3	BME	c	603	-	3,3,3	0.18	0	1,2,2	0.33	0
4	HEZ	L	601	-	7,7,7	0.21	0	6,6,6	0.12	0
3	BME	J	601	-	3,3,3	0.23	0	1,2,2	0.18	0
3	BME	E	601	-	3,3,3	0.18	0	1,2,2	0.14	0
3	BME	G	603	-	3,3,3	0.14	0	1,2,2	0.21	0
4	HEZ	B	603	-	7,7,7	0.28	0	6,6,6	0.13	0
4	HEZ	B	604	-	7,7,7	0.19	0	6,6,6	0.12	0
3	BME	Z	601	-	3,3,3	0.23	0	1,2,2	0.03	0
4	HEZ	P	603	-	7,7,7	0.27	0	6,6,6	0.15	0
4	HEZ	T	602	-	7,7,7	0.25	0	6,6,6	0.12	0
4	HEZ	A	603	-	7,7,7	0.12	0	6,6,6	0.12	0
3	BME	P	601	-	3,3,3	0.27	0	1,2,2	0.13	0
3	BME	P	602	-	3,3,3	0.24	0	1,2,2	0.19	0
3	BME	Q	603	-	3,3,3	0.14	0	1,2,2	0.10	0
3	BME	E	603	-	3,3,3	0.17	0	1,2,2	0.11	0
3	BME	G	604	-	3,3,3	0.17	0	1,2,2	0.22	0
3	BME	c	601	-	3,3,3	0.22	0	1,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BME	R	602	-	3,3,3	0.18	0	1,2,2	0.06	0
3	BME	M	601	-	3,3,3	0.26	0	1,2,2	0.50	0
3	BME	B	602	-	3,3,3	0.14	0	1,2,2	0.23	0
3	BME	O	602	-	3,3,3	0.24	0	1,2,2	0.20	0
3	BME	G	601	-	3,3,3	0.23	0	1,2,2	0.18	0
4	HEZ	c	604	-	7,7,7	0.23	0	6,6,6	0.14	0
3	BME	N	601	-	3,3,3	0.15	0	1,2,2	0.10	0
4	HEZ	Z	602	-	7,7,7	0.19	0	6,6,6	0.12	0
3	BME	D	602	-	3,3,3	0.18	0	1,2,2	0.11	0
3	BME	Q	601	-	3,3,3	0.18	0	1,2,2	0.08	0
4	HEZ	Y	602	-	7,7,7	0.20	0	6,6,6	0.12	0
4	HEZ	V	603	-	7,7,7	0.09	0	6,6,6	0.11	0
4	HEZ	K	602	-	7,7,7	0.15	0	6,6,6	0.14	0
3	BME	c	602	-	3,3,3	0.16	0	1,2,2	0.02	0
4	HEZ	c	606	-	7,7,7	0.26	0	6,6,6	0.13	0
4	HEZ	C	602	-	7,7,7	0.17	0	6,6,6	0.12	0
4	HEZ	J	602	-	7,7,7	0.25	0	6,6,6	0.12	0
4	HEZ	G	605	-	7,7,7	0.18	0	6,6,6	0.11	0
4	HEZ	V	602	-	7,7,7	0.09	0	6,6,6	0.13	0
3	BME	D	601	-	3,3,3	0.25	0	1,2,2	0.20	0
3	BME	D	603	-	3,3,3	0.19	0	1,2,2	0.25	0
4	HEZ	E	604	-	7,7,7	0.09	0	6,6,6	0.13	0
4	HEZ	I	602	-	7,7,7	0.12	0	6,6,6	0.11	0
3	BME	C	601	-	3,3,3	0.18	0	1,2,2	0.15	0
4	HEZ	A	602	-	7,7,7	0.08	0	6,6,6	0.11	0
4	HEZ	D	604	-	7,7,7	0.10	0	6,6,6	0.13	0
3	BME	T	601	-	3,3,3	0.13	0	1,2,2	0.11	0
4	HEZ	F	602	-	7,7,7	0.19	0	6,6,6	0.13	0
4	HEZ	a	602	-	7,7,7	0.18	0	6,6,6	0.13	0
3	BME	Y	601	-	3,3,3	0.18	0	1,2,2	0.08	0
3	BME	G	602	-	3,3,3	0.16	0	1,2,2	0.09	0
3	BME	X	601	-	3,3,3	0.31	0	1,2,2	0.26	0
3	BME	K	601	-	3,3,3	0.13	0	1,2,2	0.20	0
4	HEZ	T	603	-	7,7,7	0.07	0	6,6,6	0.13	0
3	BME	Q	602	-	3,3,3	0.21	0	1,2,2	0.23	0
4	HEZ	b	602	-	7,7,7	0.15	0	6,6,6	0.14	0
4	HEZ	W	601	-	7,7,7	0.13	0	6,6,6	0.13	0
4	HEZ	M	602	-	7,7,7	0.16	0	6,6,6	0.12	0
3	BME	O	601	-	3,3,3	0.24	0	1,2,2	0.26	0
3	BME	X	602	-	3,3,3	0.19	0	1,2,2	0.11	0
4	HEZ	R	603	-	7,7,7	0.17	0	6,6,6	0.13	0
4	HEZ	E	606	-	7,7,7	0.16	0	6,6,6	0.14	0
4	HEZ	R	604	-	7,7,7	0.19	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BME	H	601	-	3,3,3	0.30	0	1,2,2	0.29	0
3	BME	U	601	-	3,3,3	0.33	0	1,2,2	0.24	0
3	BME	a	601	-	3,3,3	0.18	0	1,2,2	0.04	0
3	BME	O	603	-	3,3,3	0.22	0	1,2,2	0.11	0
4	HEZ	X	603	-	7,7,7	0.11	0	6,6,6	0.13	0
3	BME	b	601	-	3,3,3	0.18	0	1,2,2	0.05	0
3	BME	V	601	-	3,3,3	0.13	0	1,2,2	0.06	0
3	BME	E	602	-	3,3,3	0.22	0	1,2,2	0.19	0
4	HEZ	D	605	-	7,7,7	0.15	0	6,6,6	0.13	0
3	BME	B	601	-	3,3,3	0.41	0	1,2,2	0.23	0
4	HEZ	I	601	-	7,7,7	0.16	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEZ	E	605	-	-	4/5/5/5	-
3	BME	F	601	-	-	0/1/1/1	-
4	HEZ	F	603	-	-	4/5/5/5	-
4	HEZ	W	602	-	-	2/5/5/5	-
3	BME	A	601	-	-	1/1/1/1	-
4	HEZ	H	602	-	-	4/5/5/5	-
4	HEZ	N	602	-	-	1/5/5/5	-
4	HEZ	Q	604	-	-	4/5/5/5	-
4	HEZ	c	605	-	-	4/5/5/5	-
4	HEZ	O	605	-	-	2/5/5/5	-
4	HEZ	O	604	-	-	3/5/5/5	-
3	BME	U	602	-	-	1/1/1/1	-
4	HEZ	U	604	-	-	4/5/5/5	-
3	BME	U	603	-	-	0/1/1/1	-
3	BME	R	601	-	-	0/1/1/1	-
3	BME	c	603	-	-	1/1/1/1	-
4	HEZ	L	601	-	-	4/5/5/5	-
3	BME	J	601	-	-	0/1/1/1	-
3	BME	E	601	-	-	0/1/1/1	-
3	BME	G	603	-	-	1/1/1/1	-
4	HEZ	B	603	-	-	5/5/5/5	-
4	HEZ	B	604	-	-	4/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BME	Z	601	-	-	0/1/1/1	-
4	HEZ	P	603	-	-	4/5/5/5	-
4	HEZ	T	602	-	-	0/5/5/5	-
4	HEZ	A	603	-	-	3/5/5/5	-
3	BME	P	601	-	-	1/1/1/1	-
3	BME	P	602	-	-	1/1/1/1	-
3	BME	Q	603	-	-	0/1/1/1	-
3	BME	E	603	-	-	1/1/1/1	-
3	BME	G	604	-	-	1/1/1/1	-
3	BME	c	601	-	-	0/1/1/1	-
3	BME	R	602	-	-	0/1/1/1	-
3	BME	M	601	-	-	1/1/1/1	-
3	BME	B	602	-	-	1/1/1/1	-
3	BME	O	602	-	-	0/1/1/1	-
3	BME	G	601	-	-	0/1/1/1	-
4	HEZ	c	604	-	-	2/5/5/5	-
3	BME	N	601	-	-	1/1/1/1	-
4	HEZ	Z	602	-	-	4/5/5/5	-
3	BME	D	602	-	-	0/1/1/1	-
3	BME	Q	601	-	-	1/1/1/1	-
4	HEZ	Y	602	-	-	2/5/5/5	-
4	HEZ	V	603	-	-	3/5/5/5	-
4	HEZ	K	602	-	-	0/5/5/5	-
3	BME	c	602	-	-	0/1/1/1	-
4	HEZ	c	606	-	-	1/5/5/5	-
4	HEZ	C	602	-	-	4/5/5/5	-
4	HEZ	J	602	-	-	4/5/5/5	-
4	HEZ	G	605	-	-	3/5/5/5	-
4	HEZ	V	602	-	-	3/5/5/5	-
3	BME	D	601	-	-	1/1/1/1	-
3	BME	D	603	-	-	1/1/1/1	-
4	HEZ	E	604	-	-	3/5/5/5	-
4	HEZ	I	602	-	-	1/5/5/5	-
3	BME	C	601	-	-	1/1/1/1	-
4	HEZ	A	602	-	-	4/5/5/5	-
4	HEZ	D	604	-	-	3/5/5/5	-
3	BME	T	601	-	-	0/1/1/1	-
4	HEZ	F	602	-	-	3/5/5/5	-
4	HEZ	a	602	-	-	3/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BME	Y	601	-	-	1/1/1/1	-
3	BME	G	602	-	-	1/1/1/1	-
3	BME	X	601	-	-	0/1/1/1	-
3	BME	K	601	-	-	0/1/1/1	-
4	HEZ	T	603	-	-	3/5/5/5	-
3	BME	Q	602	-	-	1/1/1/1	-
4	HEZ	b	602	-	-	2/5/5/5	-
4	HEZ	W	601	-	-	2/5/5/5	-
4	HEZ	M	602	-	-	3/5/5/5	-
3	BME	O	601	-	-	1/1/1/1	-
3	BME	X	602	-	-	0/1/1/1	-
4	HEZ	R	603	-	-	2/5/5/5	-
4	HEZ	E	606	-	-	0/5/5/5	-
4	HEZ	R	604	-	-	3/5/5/5	-
3	BME	H	601	-	-	0/1/1/1	-
3	BME	U	601	-	-	0/1/1/1	-
3	BME	a	601	-	-	1/1/1/1	-
3	BME	O	603	-	-	1/1/1/1	-
4	HEZ	X	603	-	-	2/5/5/5	-
3	BME	b	601	-	-	0/1/1/1	-
3	BME	V	601	-	-	1/1/1/1	-
3	BME	E	602	-	-	1/1/1/1	-
4	HEZ	D	605	-	-	3/5/5/5	-
3	BME	B	601	-	-	1/1/1/1	-
4	HEZ	I	601	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (141) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	BME	O1-C1-C2-S2
3	D	603	BME	O1-C1-C2-S2
3	E	602	BME	O1-C1-C2-S2
3	E	603	BME	O1-C1-C2-S2
3	G	602	BME	O1-C1-C2-S2
3	G	604	BME	O1-C1-C2-S2
3	O	603	BME	O1-C1-C2-S2

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Mol	Chain	Res	Type	Atoms
3	P	601	BME	O1-C1-C2-S2
3	P	602	BME	O1-C1-C2-S2
3	Q	601	BME	O1-C1-C2-S2
3	U	602	BME	O1-C1-C2-S2
3	V	601	BME	O1-C1-C2-S2
3	a	601	BME	O1-C1-C2-S2
3	c	603	BME	O1-C1-C2-S2
4	R	604	HEZ	C3-C4-C5-C6
4	W	602	HEZ	C3-C4-C5-C6
4	c	605	HEZ	C4-C5-C6-O6
4	F	603	HEZ	C2-C3-C4-C5
4	J	602	HEZ	C2-C3-C4-C5
4	C	602	HEZ	C2-C3-C4-C5
4	F	603	HEZ	C1-C2-C3-C4
4	O	604	HEZ	C3-C4-C5-C6
4	E	604	HEZ	C2-C3-C4-C5
4	C	602	HEZ	C3-C4-C5-C6
4	Q	604	HEZ	C3-C4-C5-C6
4	A	603	HEZ	C3-C4-C5-C6
4	D	605	HEZ	C3-C4-C5-C6
4	c	605	HEZ	C3-C4-C5-C6
4	X	603	HEZ	C1-C2-C3-C4
4	Y	602	HEZ	C2-C3-C4-C5
4	B	603	HEZ	C1-C2-C3-C4
4	F	603	HEZ	C3-C4-C5-C6
4	H	602	HEZ	C1-C2-C3-C4
4	L	601	HEZ	C3-C4-C5-C6
4	M	602	HEZ	C1-C2-C3-C4
4	M	602	HEZ	C3-C4-C5-C6
4	J	602	HEZ	C1-C2-C3-C4
4	T	603	HEZ	C1-C2-C3-C4
4	a	602	HEZ	C1-C2-C3-C4
4	H	602	HEZ	C3-C4-C5-C6
4	I	601	HEZ	C3-C4-C5-C6
4	U	604	HEZ	C3-C4-C5-C6
4	F	602	HEZ	C3-C4-C5-C6
4	P	603	HEZ	C1-C2-C3-C4
4	c	606	HEZ	C3-C4-C5-C6
4	B	603	HEZ	C2-C3-C4-C5
4	Q	604	HEZ	C2-C3-C4-C5
3	M	601	BME	O1-C1-C2-S2
3	N	601	BME	O1-C1-C2-S2

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Mol	Chain	Res	Type	Atoms
3	O	601	BME	O1-C1-C2-S2
4	A	602	HEZ	C1-C2-C3-C4
4	c	605	HEZ	C1-C2-C3-C4
4	W	601	HEZ	C1-C2-C3-C4
4	W	601	HEZ	C2-C3-C4-C5
4	Z	602	HEZ	C1-C2-C3-C4
4	W	602	HEZ	C2-C3-C4-C5
4	X	603	HEZ	C2-C3-C4-C5
4	A	603	HEZ	C1-C2-C3-C4
4	E	604	HEZ	C1-C2-C3-C4
4	E	605	HEZ	C1-C2-C3-C4
4	B	604	HEZ	C1-C2-C3-C4
4	J	602	HEZ	C3-C4-C5-C6
4	G	605	HEZ	C3-C4-C5-C6
4	b	602	HEZ	C3-C4-C5-C6
4	E	605	HEZ	O1-C1-C2-C3
4	A	602	HEZ	C4-C5-C6-O6
4	D	604	HEZ	O1-C1-C2-C3
4	G	605	HEZ	O1-C1-C2-C3
4	I	601	HEZ	O1-C1-C2-C3
4	R	603	HEZ	O1-C1-C2-C3
4	c	604	HEZ	O1-C1-C2-C3
4	A	602	HEZ	C3-C4-C5-C6
4	O	604	HEZ	C1-C2-C3-C4
4	V	603	HEZ	C1-C2-C3-C4
4	B	604	HEZ	C4-C5-C6-O6
4	D	605	HEZ	C4-C5-C6-O6
4	J	602	HEZ	O1-C1-C2-C3
4	O	604	HEZ	O1-C1-C2-C3
4	P	603	HEZ	C4-C5-C6-O6
4	Q	604	HEZ	C4-C5-C6-O6
4	T	603	HEZ	O1-C1-C2-C3
4	a	602	HEZ	C4-C5-C6-O6
4	A	602	HEZ	O1-C1-C2-C3
4	B	603	HEZ	C4-C5-C6-O6
4	D	604	HEZ	C4-C5-C6-O6
4	H	602	HEZ	O1-C1-C2-C3
4	L	601	HEZ	O1-C1-C2-C3
4	L	601	HEZ	C4-C5-C6-O6
4	R	603	HEZ	C4-C5-C6-O6
4	V	602	HEZ	O1-C1-C2-C3
4	N	602	HEZ	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	D	605	HEZ	C2-C3-C4-C5
4	c	604	HEZ	C2-C3-C4-C5
4	O	605	HEZ	C1-C2-C3-C4
4	M	602	HEZ	O1-C1-C2-C3
4	U	604	HEZ	C4-C5-C6-O6
4	C	602	HEZ	C1-C2-C3-C4
4	E	604	HEZ	C3-C4-C5-C6
4	R	604	HEZ	C1-C2-C3-C4
4	A	603	HEZ	C2-C3-C4-C5
3	A	601	BME	O1-C1-C2-S2
3	B	602	BME	O1-C1-C2-S2
3	G	603	BME	O1-C1-C2-S2
3	Q	602	BME	O1-C1-C2-S2
4	B	603	HEZ	C3-C4-C5-C6
4	I	602	HEZ	C4-C5-C6-O6
4	P	603	HEZ	C3-C4-C5-C6
4	Z	602	HEZ	C2-C3-C4-C5
4	D	604	HEZ	C3-C4-C5-C6
4	C	602	HEZ	O1-C1-C2-C3
4	F	603	HEZ	O1-C1-C2-C3
4	Z	602	HEZ	O1-C1-C2-C3
3	B	601	BME	O1-C1-C2-S2
3	D	601	BME	O1-C1-C2-S2
4	Q	604	HEZ	C1-C2-C3-C4
4	V	603	HEZ	O1-C1-C2-C3
4	c	605	HEZ	O1-C1-C2-C3
4	U	604	HEZ	O1-C1-C2-C3
4	G	605	HEZ	C4-C5-C6-O6
4	B	603	HEZ	O1-C1-C2-C3
4	V	603	HEZ	C2-C3-C4-C5
4	E	605	HEZ	C2-C3-C4-C5
4	P	603	HEZ	C2-C3-C4-C5
4	U	604	HEZ	C2-C3-C4-C5
4	F	602	HEZ	O1-C1-C2-C3
4	a	602	HEZ	C2-C3-C4-C5
4	R	604	HEZ	C4-C5-C6-O6
4	Y	602	HEZ	O1-C1-C2-C3
4	L	601	HEZ	C2-C3-C4-C5
3	Y	601	BME	O1-C1-C2-S2
4	O	605	HEZ	C3-C4-C5-C6
4	V	602	HEZ	C4-C5-C6-O6
4	T	603	HEZ	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	b	602	HEZ	C2-C3-C4-C5
4	V	602	HEZ	C1-C2-C3-C4
4	B	604	HEZ	C3-C4-C5-C6
4	B	604	HEZ	C2-C3-C4-C5
4	E	605	HEZ	C4-C5-C6-O6
4	Z	602	HEZ	C3-C4-C5-C6
4	H	602	HEZ	C2-C3-C4-C5
4	F	602	HEZ	C2-C3-C4-C5

There are no ring outliers.

21 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	602	HEZ	1	0
4	Q	604	HEZ	1	0
4	U	604	HEZ	1	0
3	G	603	BME	1	0
4	B	604	HEZ	2	0
4	P	603	HEZ	1	0
3	Q	603	BME	1	0
3	c	601	BME	1	0
3	M	601	BME	1	0
3	O	602	BME	1	0
3	Q	601	BME	2	0
4	Y	602	HEZ	1	0
4	K	602	HEZ	1	0
3	c	602	BME	1	0
4	E	604	HEZ	1	0
4	D	604	HEZ	1	0
3	K	601	BME	2	0
4	R	603	HEZ	1	0
4	R	604	HEZ	1	0
4	X	603	HEZ	1	0
3	E	602	BME	1	0

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(Å ²)	Q<0.9
1	A	524/548 (95%)	0.06	16 (3%) 51 30	42, 76, 141, 183	0
1	B	524/548 (95%)	-0.16	3 (0%) 85 71	37, 66, 119, 161	0
1	C	524/548 (95%)	0.01	12 (2%) 61 39	37, 73, 143, 194	0
1	F	523/548 (95%)	0.06	18 (3%) 48 28	42, 80, 151, 217	0
1	G	524/548 (95%)	0.04	14 (2%) 56 34	42, 78, 152, 189	0
1	H	524/548 (95%)	-0.37	1 (0%) 92 84	35, 58, 89, 141	0
1	I	523/548 (95%)	-0.49	2 (0%) 89 77	33, 53, 80, 144	0
1	J	524/548 (95%)	-0.32	5 (0%) 79 60	37, 63, 101, 159	0
1	M	524/548 (95%)	-0.13	7 (1%) 74 54	39, 72, 111, 143	0
1	N	524/548 (95%)	-0.29	0 100 100	36, 63, 93, 136	0
1	P	524/548 (95%)	-0.25	2 (0%) 89 77	38, 69, 112, 146	0
1	Q	524/548 (95%)	-0.09	4 (0%) 82 66	35, 70, 125, 153	0
1	T	524/548 (95%)	-0.30	3 (0%) 85 71	42, 71, 99, 152	0
1	U	524/548 (95%)	-0.42	0 100 100	36, 60, 95, 133	0
1	Y	524/548 (95%)	0.05	21 (4%) 43 25	37, 69, 148, 200	0
1	a	524/548 (95%)	0.00	11 (2%) 63 41	36, 73, 147, 193	0
1	b	524/548 (95%)	-0.13	4 (0%) 82 66	41, 77, 126, 159	0
2	D	525/548 (95%)	0.09	20 (3%) 44 26	38, 74, 159, 225	0
2	E	525/548 (95%)	-0.05	10 (1%) 66 44	39, 72, 151, 212	0
2	K	525/548 (95%)	0.13	26 (4%) 35 20	39, 84, 163, 194	0
2	L	525/548 (95%)	0.00	10 (1%) 66 44	41, 80, 144, 173	0
2	O	525/548 (95%)	-0.41	1 (0%) 92 84	38, 60, 90, 144	0
2	R	525/548 (95%)	-0.16	2 (0%) 89 77	41, 74, 114, 144	0
2	V	525/548 (95%)	0.01	6 (1%) 77 58	43, 82, 129, 168	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	525/548 (95%)	-0.02	4 (0%) 82 66	43, 82, 139, 170	0
2	X	525/548 (95%)	-0.01	11 (2%) 63 41	39, 74, 155, 223	0
2	Z	525/548 (95%)	-0.29	3 (0%) 85 71	34, 63, 116, 154	0
2	c	525/548 (95%)	-0.39	2 (0%) 89 77	42, 60, 89, 143	0
All	All	14681/15344 (95%)	-0.14	218 (1%) 71 50	33, 69, 136, 225	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	271	VAL	4.7
1	C	237	LEU	4.5
1	C	271	VAL	4.4
1	A	239	ALA	4.3
2	L	271	VAL	4.3
2	K	237	LEU	4.2
1	A	314	LEU	4.0
2	K	300	VAL	4.0
1	F	240	VAL	3.7
1	Q	271	VAL	3.7
1	Y	237	LEU	3.7
2	E	314	LEU	3.6
1	a	271	VAL	3.5
2	V	360	TYR	3.5
1	F	243	ALA	3.4
2	K	270	ILE	3.4
2	X	233	MET	3.4
2	K	314	LEU	3.3
1	Y	239	ALA	3.3
2	E	237	LEU	3.3
1	A	292	ILE	3.3
2	Z	270	ILE	3.3
1	F	273	VAL	3.3
2	L	302	SER	3.2
2	X	271	VAL	3.2
1	Y	309	LEU	3.2
2	X	237	LEU	3.2
1	F	270	ILE	3.1
1	B	271	VAL	3.1
2	K	248	LEU	3.1
1	G	272	LYS	3.1
2	E	239	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	X	270	ILE	3.1
2	E	526	LYS	3.1
2	V	284	ARG	3.1
2	D	314	LEU	3.1
2	D	239	ALA	3.0
2	D	236	VAL	3.0
1	Y	233	MET	3.0
2	K	233	MET	3.0
1	C	241	ALA	3.0
2	K	223	ALA	3.0
2	V	270	ILE	2.9
1	a	332	ILE	2.9
1	Y	314	LEU	2.9
2	X	272	LYS	2.9
1	A	237	LEU	2.9
1	G	262	LEU	2.9
2	K	305	ILE	2.8
1	a	240	VAL	2.8
1	F	237	LEU	2.8
2	X	223	ALA	2.8
1	G	220	ILE	2.8
1	J	271	VAL	2.7
2	D	240	VAL	2.7
1	Q	309	LEU	2.7
1	G	264	VAL	2.7
2	L	213	VAL	2.7
2	X	240	VAL	2.7
2	X	264	VAL	2.7
1	a	314	LEU	2.7
1	G	270	ILE	2.7
1	Y	301	ILE	2.7
2	K	299	THR	2.7
2	E	272	LYS	2.7
2	K	215	LEU	2.7
1	P	270	ILE	2.7
1	Y	300	VAL	2.7
2	D	271	VAL	2.7
2	D	300	VAL	2.7
2	L	275	ALA	2.7
1	B	44	PHE	2.7
2	D	305	ILE	2.7
2	X	309	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	Y	255	GLU	2.6
2	D	275	ALA	2.6
1	G	237	LEU	2.6
1	C	44	PHE	2.6
1	F	233	MET	2.6
1	A	336	VAL	2.6
1	Y	240	VAL	2.6
2	D	264	VAL	2.6
1	T	477	GLY	2.6
1	F	241	ALA	2.6
1	Y	262	LEU	2.6
2	K	239	ALA	2.6
1	b	44	PHE	2.6
1	H	44	PHE	2.5
2	R	305	ILE	2.5
2	D	247	LEU	2.5
1	a	270	ILE	2.5
2	D	267	MET	2.5
2	E	44	PHE	2.5
2	L	227	ILE	2.5
1	a	44	PHE	2.5
1	b	314	LEU	2.5
2	E	271	VAL	2.5
1	G	210	THR	2.5
1	F	204	PHE	2.5
2	c	44	PHE	2.5
1	C	272	LYS	2.5
1	A	343	GLN	2.5
1	A	309	LEU	2.5
1	C	236	VAL	2.5
1	Y	254	VAL	2.5
1	A	342	ILE	2.5
1	C	240	VAL	2.4
1	A	229	ASN	2.4
2	E	270	ILE	2.4
1	J	44	PHE	2.4
1	Y	266	THR	2.4
1	a	272	LYS	2.4
1	F	88	GLY	2.4
1	G	221	LEU	2.4
1	b	233	MET	2.4
1	P	44	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	203	TYR	2.4
2	W	271	VAL	2.4
1	C	249	ILE	2.4
2	D	249	ILE	2.4
2	E	233	MET	2.4
1	C	273	VAL	2.4
1	Y	241	ALA	2.4
1	a	265	ASN	2.4
2	D	299	THR	2.4
2	Z	237	LEU	2.3
2	K	236	VAL	2.3
1	I	44	PHE	2.3
1	Y	243	ALA	2.3
2	D	274	ALA	2.3
1	B	266	THR	2.3
2	K	234	LEU	2.3
1	a	230	ILE	2.3
2	K	219	PHE	2.3
1	F	314	LEU	2.3
1	F	272	LYS	2.3
1	G	526	LYS	2.3
2	D	272	LYS	2.3
2	K	309	LEU	2.3
1	J	266	THR	2.3
1	Y	271	VAL	2.3
2	X	236	VAL	2.3
1	G	314	LEU	2.3
1	Y	526	LYS	2.3
1	Y	236	VAL	2.2
1	G	44	PHE	2.2
1	A	251	ALA	2.2
2	W	389	MET	2.2
1	C	247	LEU	2.2
1	C	233	MET	2.2
2	D	200	LEU	2.2
1	A	296	THR	2.2
1	I	266	THR	2.2
2	K	204	PHE	2.2
1	C	275	ALA	2.2
1	G	274	ALA	2.2
1	F	294	THR	2.2
2	K	301	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	T	206	ASN	2.2
1	A	320	ALA	2.2
1	F	239	ALA	2.2
1	M	34	LYS	2.2
1	M	372	LEU	2.2
2	L	234	LEU	2.2
2	V	34	LYS	2.2
2	X	526	LYS	2.2
1	A	235	PRO	2.2
2	E	43	SER	2.2
2	c	270	ILE	2.2
1	A	240	VAL	2.2
1	Y	273	VAL	2.2
2	K	266	THR	2.1
1	T	44	PHE	2.1
2	K	44	PHE	2.1
2	Z	239	ALA	2.1
2	D	263	VAL	2.1
1	M	44	PHE	2.1
2	O	44	PHE	2.1
1	F	259	LEU	2.1
2	K	259	LEU	2.1
2	K	317	LEU	2.1
2	W	272	LYS	2.1
1	F	236	VAL	2.1
1	b	266	THR	2.1
1	J	272	LYS	2.1
1	M	373	ALA	2.1
2	L	301	ILE	2.1
1	a	264	VAL	2.1
1	A	233	MET	2.1
2	L	244	GLY	2.1
1	Q	526	LYS	2.1
2	K	262	LEU	2.1
1	M	223	ALA	2.1
2	L	203	TYR	2.1
2	V	349	ILE	2.1
1	F	458	CYS	2.1
1	Y	364	LYS	2.1
1	M	299	THR	2.0
1	Y	275	ALA	2.0
1	a	241	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	338	GLU	2.0
2	K	227	ILE	2.0
2	L	325	ILE	2.0
1	G	236	VAL	2.0
1	G	309	LEU	2.0
1	Q	44	PHE	2.0
2	D	237	LEU	2.0
2	K	289	LEU	2.0
2	W	314	LEU	2.0
2	D	223	ALA	2.0
2	V	243	ALA	2.0
1	Y	249	ILE	2.0
1	F	488	MET	2.0
1	J	526	LYS	2.0
1	M	254	VAL	2.0
2	K	254	VAL	2.0
2	D	44	PHE	2.0
2	R	44	PHE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	A	43	10/11	0.56	0.16	109,129,159,163	0
1	SEP	H	43	10/11	0.57	0.16	102,132,157,160	0
1	SEP	I	43	10/11	0.58	0.15	111,138,166,174	0
1	SEP	M	43	10/11	0.60	0.17	101,123,141,162	0
1	SEP	U	43	10/11	0.60	0.17	107,139,163,169	0
1	SEP	T	43	10/11	0.61	0.16	113,132,163,165	0
1	SEP	N	43	10/11	0.61	0.15	102,117,129,135	0
1	SEP	J	43	10/11	0.63	0.14	106,127,161,164	0
1	SEP	G	43	10/11	0.64	0.19	120,138,154,168	0
1	SEP	C	43	10/11	0.66	0.15	106,131,158,161	0
1	SEP	Q	43	10/11	0.67	0.17	102,138,164,176	0
1	SEP	b	43	10/11	0.68	0.15	115,137,161,174	0
1	SEP	F	43	10/11	0.70	0.15	107,129,145,149	0
1	SEP	a	43	10/11	0.72	0.15	114,125,142,148	0
1	SEP	Y	43	10/11	0.74	0.17	107,126,139,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SEP	B	43	10/11	0.75	0.19	101,113,130,136	0
1	SEP	P	43	10/11	0.78	0.15	113,131,150,157	0

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(\AA^2)	Q<0.9
3	BME	E	602	4/4	0.57	0.19	116,142,142,145	0
3	BME	V	601	4/4	0.59	0.14	132,133,134,135	0
3	BME	G	604	4/4	0.70	0.23	99,107,113,125	0
3	BME	G	603	4/4	0.73	0.14	78,87,94,109	0
4	HEZ	V	603	8/8	0.78	0.19	96,109,115,116	0
5	MG	N	603	1/1	0.78	0.10	80,80,80,80	0
3	BME	U	603	4/4	0.79	0.19	98,100,107,122	0
3	BME	O	603	4/4	0.80	0.20	95,109,113,115	0
3	BME	D	602	4/4	0.81	0.12	102,104,104,106	0
4	HEZ	B	604	8/8	0.83	0.23	79,107,110,110	0
5	MG	c	607	1/1	0.83	0.09	76,76,76,76	0
5	MG	G	606	1/1	0.84	0.13	110,110,110,110	0
3	BME	R	602	4/4	0.84	0.17	106,107,108,112	0
3	BME	X	602	4/4	0.84	0.19	93,104,113,116	0
3	BME	c	602	4/4	0.85	0.14	71,84,85,86	0
4	HEZ	D	605	8/8	0.85	0.19	79,97,104,107	0
3	BME	Q	603	4/4	0.86	0.14	79,79,84,94	0
4	HEZ	O	605	8/8	0.86	0.20	79,96,112,114	0
3	BME	E	601	4/4	0.87	0.12	103,115,119,121	0
4	HEZ	V	602	8/8	0.87	0.18	76,87,109,110	0
4	HEZ	A	603	8/8	0.87	0.17	98,103,107,107	0
4	HEZ	F	603	8/8	0.88	0.20	79,85,90,93	0
3	BME	c	603	4/4	0.88	0.16	57,69,75,97	0
4	HEZ	T	602	8/8	0.88	0.16	60,86,109,114	0
5	MG	T	604	1/1	0.88	0.14	94,94,94,94	0
5	MG	b	603	1/1	0.88	0.11	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BME	c	601	4/4	0.88	0.11	72,87,88,99	0
3	BME	Q	602	4/4	0.89	0.22	70,74,89,116	0
3	BME	C	601	4/4	0.89	0.19	69,78,81,98	0
4	HEZ	E	606	8/8	0.89	0.15	77,82,85,87	0
4	HEZ	B	603	8/8	0.89	0.18	56,73,91,92	0
4	HEZ	c	606	8/8	0.89	0.17	77,84,88,90	0
3	BME	O	602	4/4	0.90	0.20	87,91,97,97	0
4	HEZ	E	604	8/8	0.90	0.12	61,64,73,78	0
4	HEZ	E	605	8/8	0.90	0.15	61,66,81,89	0
4	HEZ	C	602	8/8	0.91	0.12	56,63,82,94	0
3	BME	G	601	4/4	0.91	0.14	70,73,74,82	0
4	HEZ	G	605	8/8	0.91	0.12	67,77,83,85	0
4	HEZ	H	602	8/8	0.91	0.12	59,63,67,71	0
3	BME	X	601	4/4	0.91	0.16	55,68,76,86	0
4	HEZ	P	603	8/8	0.91	0.14	46,65,88,91	0
5	MG	U	605	1/1	0.91	0.08	77,77,77,77	0
4	HEZ	R	604	8/8	0.91	0.14	67,87,94,96	0
3	BME	P	601	4/4	0.91	0.15	62,69,76,83	0
4	HEZ	c	604	8/8	0.92	0.12	53,73,86,90	0
4	HEZ	c	605	8/8	0.92	0.16	63,70,84,85	0
4	HEZ	A	602	8/8	0.92	0.13	78,81,89,96	0
5	MG	D	606	1/1	0.92	0.09	82,82,82,82	0
3	BME	D	601	4/4	0.92	0.15	77,80,80,81	0
4	HEZ	R	603	8/8	0.92	0.10	62,63,74,80	0
3	BME	M	601	4/4	0.92	0.13	54,63,67,87	0
3	BME	E	603	4/4	0.92	0.13	67,67,72,79	0
4	HEZ	K	602	8/8	0.92	0.12	59,65,79,84	0
4	HEZ	N	602	8/8	0.92	0.15	50,62,94,97	0
4	HEZ	U	604	8/8	0.93	0.12	55,58,74,81	0
4	HEZ	J	602	8/8	0.93	0.12	51,60,75,78	0
3	BME	Z	601	4/4	0.93	0.14	49,58,65,80	0
4	HEZ	W	601	8/8	0.93	0.12	61,78,92,95	0
4	HEZ	Z	602	8/8	0.93	0.16	53,62,81,84	0
4	HEZ	L	601	8/8	0.93	0.13	56,69,88,88	0
4	HEZ	M	602	8/8	0.93	0.13	64,71,83,84	0
3	BME	K	601	4/4	0.93	0.18	76,80,81,86	0
3	BME	F	601	4/4	0.93	0.12	57,65,69,83	0
5	MG	E	607	1/1	0.93	0.11	95,95,95,95	0
4	HEZ	F	602	8/8	0.93	0.12	58,62,76,83	0
4	HEZ	Q	604	8/8	0.93	0.12	53,62,80,82	0
3	BME	T	601	4/4	0.93	0.15	63,76,84,106	0
4	HEZ	D	604	8/8	0.93	0.12	60,67,82,87	0

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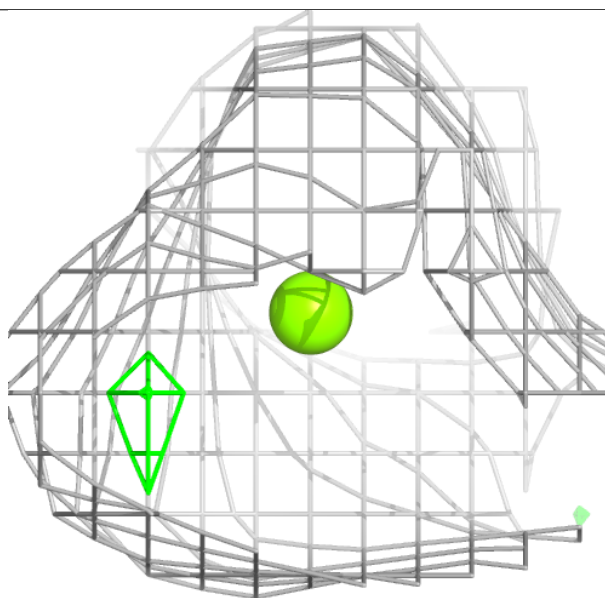
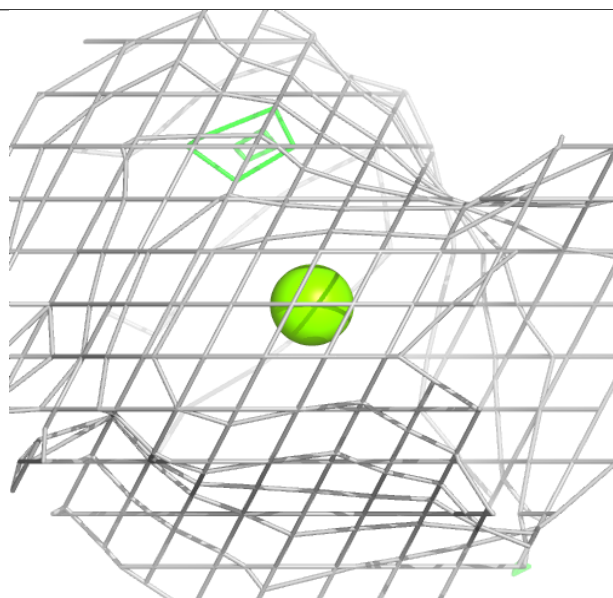
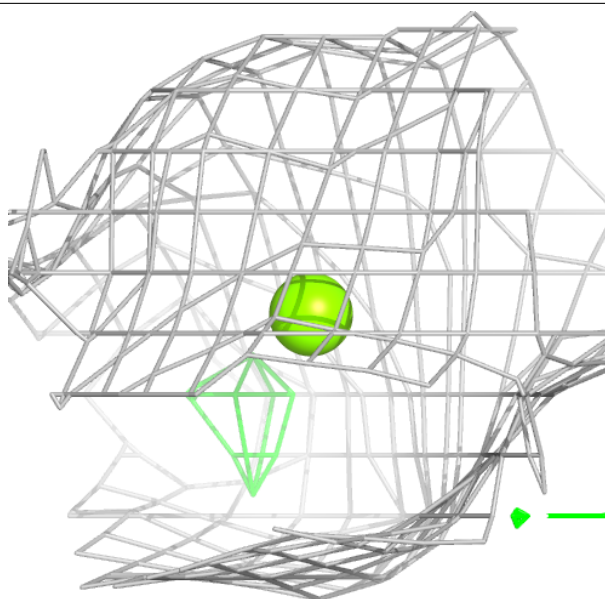
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BME	U	601	4/4	0.93	0.12	64,71,73,85	0
4	HEZ	T	603	8/8	0.93	0.16	82,91,107,110	0
3	BME	b	601	4/4	0.94	0.15	88,88,89,91	0
4	HEZ	b	602	8/8	0.94	0.14	53,71,102,108	0
3	BME	A	601	4/4	0.94	0.23	71,75,75,76	0
4	HEZ	I	602	8/8	0.94	0.16	71,77,82,93	0
3	BME	H	601	4/4	0.94	0.16	64,68,72,74	0
3	BME	J	601	4/4	0.94	0.15	81,84,87,95	0
3	BME	P	602	4/4	0.94	0.14	57,69,72,83	0
3	BME	B	601	4/4	0.94	0.16	54,60,65,82	0
3	BME	B	602	4/4	0.94	0.15	50,62,67,85	0
4	HEZ	O	604	8/8	0.94	0.14	52,59,69,76	0
3	BME	N	601	4/4	0.94	0.17	76,91,92,95	0
4	HEZ	W	602	8/8	0.94	0.12	68,82,99,101	0
4	HEZ	Y	602	8/8	0.94	0.12	54,57,75,78	0
3	BME	G	602	4/4	0.95	0.12	59,68,74,93	0
5	MG	H	603	1/1	0.95	0.15	74,74,74,74	0
5	MG	M	603	1/1	0.95	0.05	59,59,59,59	0
3	BME	O	601	4/4	0.95	0.11	62,75,83,95	0
4	HEZ	X	603	8/8	0.95	0.12	54,62,85,93	0
4	HEZ	I	601	8/8	0.95	0.11	53,60,76,84	0
5	MG	V	604	1/1	0.95	0.05	77,77,77,77	0
3	BME	R	601	4/4	0.95	0.14	82,87,88,91	0
4	HEZ	a	602	8/8	0.95	0.12	52,63,83,85	0
5	MG	H	604	1/1	0.96	0.30	39,39,39,39	0
3	BME	a	601	4/4	0.96	0.13	56,71,83,94	0
3	BME	U	602	4/4	0.96	0.16	76,78,79,86	0
3	BME	D	603	4/4	0.96	0.12	85,86,90,90	0
3	BME	Y	601	4/4	0.97	0.12	64,67,76,84	0
5	MG	F	604	1/1	0.97	0.05	87,87,87,87	0
3	BME	Q	601	4/4	0.97	0.08	57,61,64,69	0
5	MG	A	604	1/1	0.98	0.09	78,78,78,78	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.

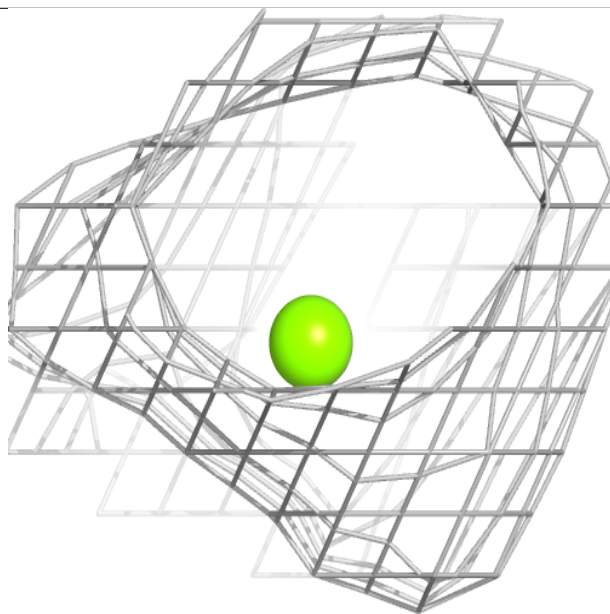
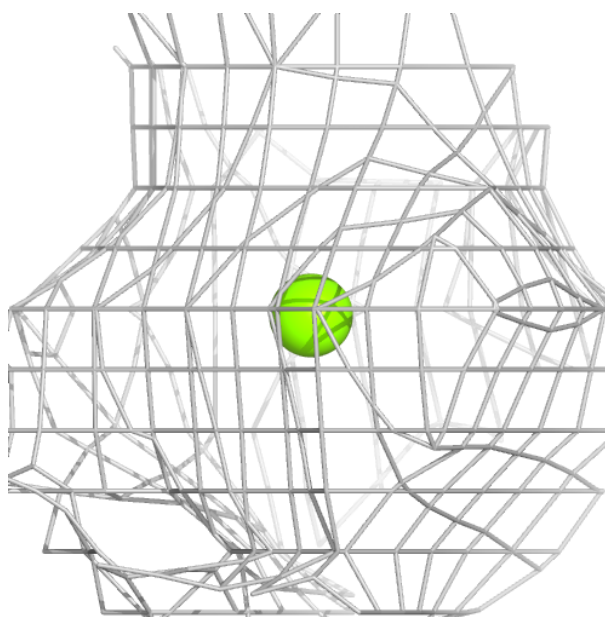
Electron density around MG N 603:

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



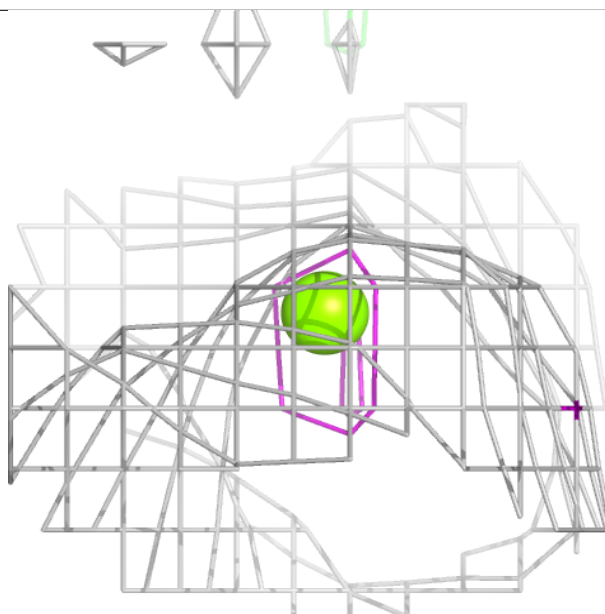
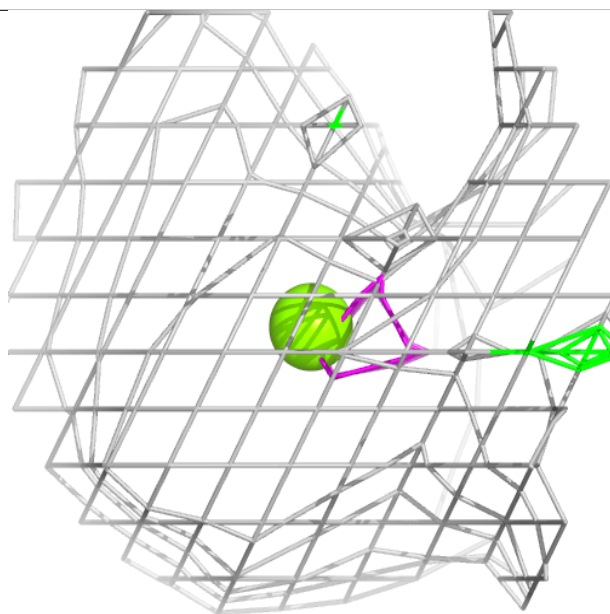
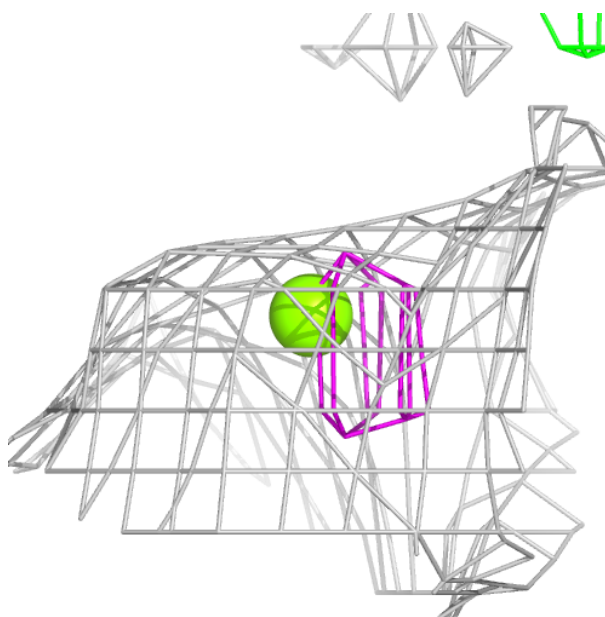
Electron density around MG c 607:

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



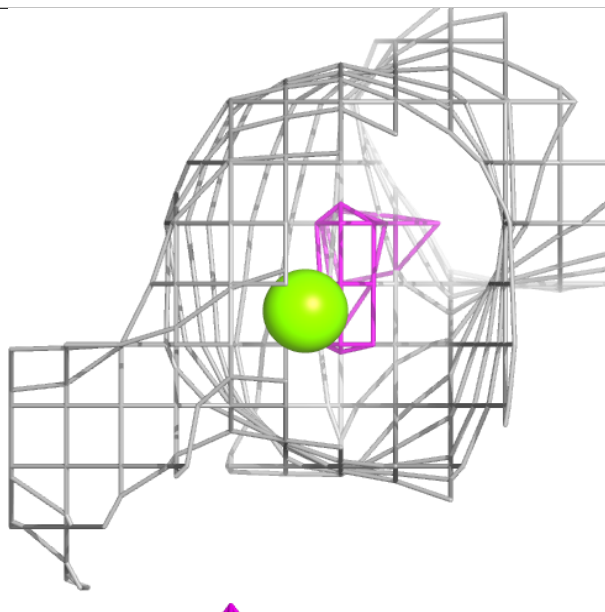
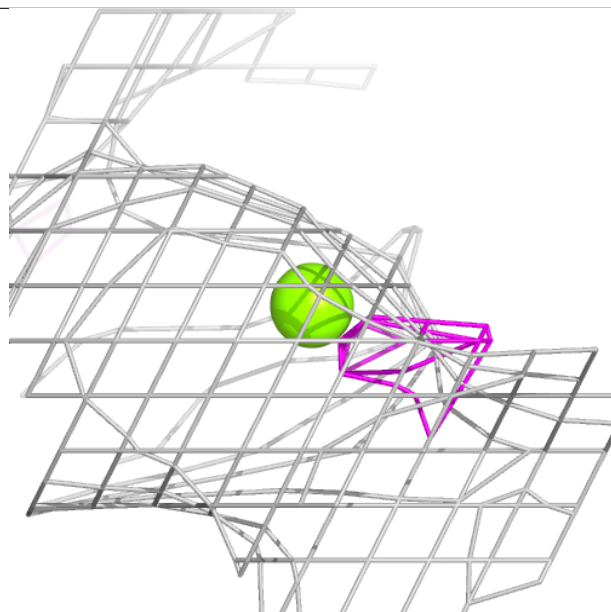
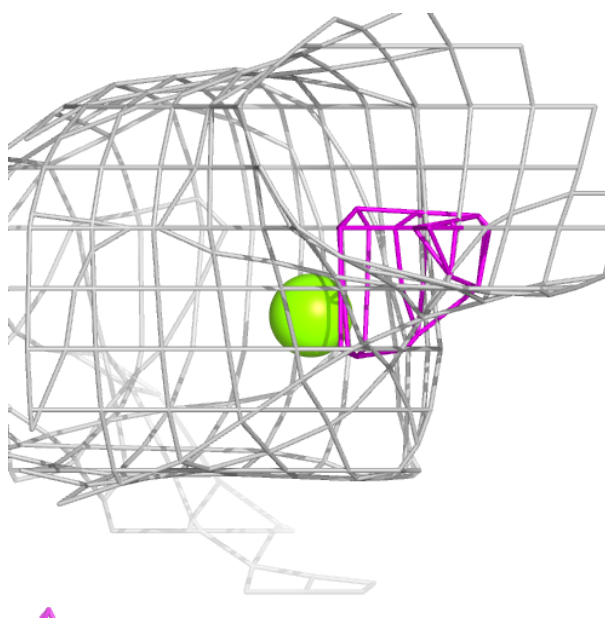
Electron density around MG G 606:

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



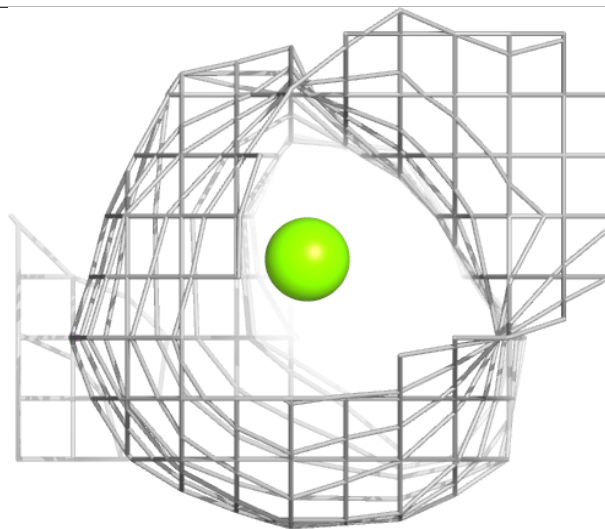
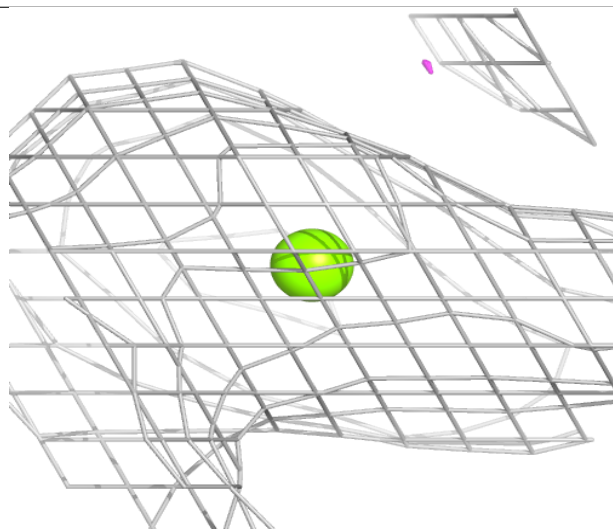
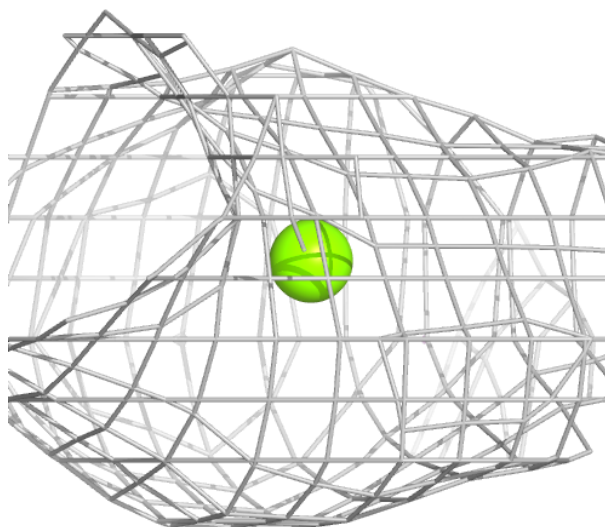
Electron density around MG T 604:

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



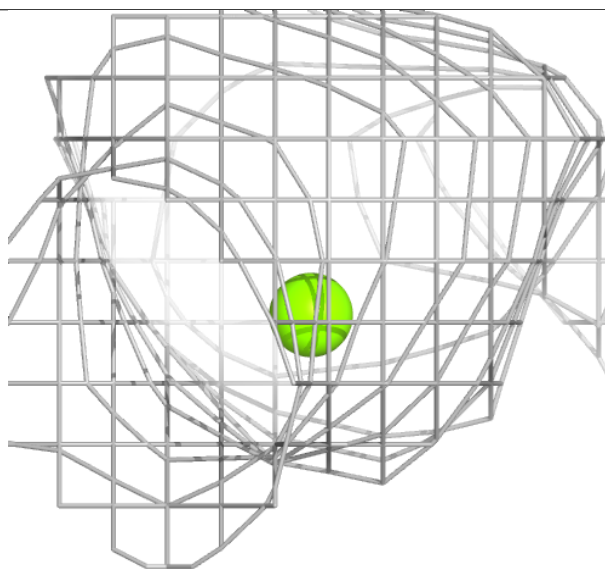
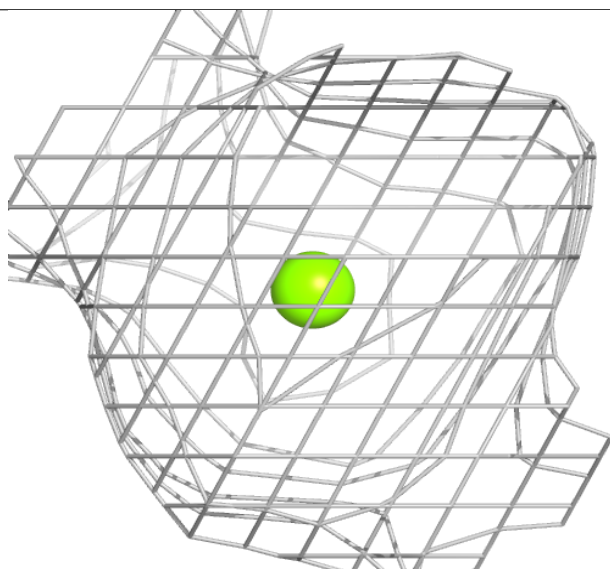
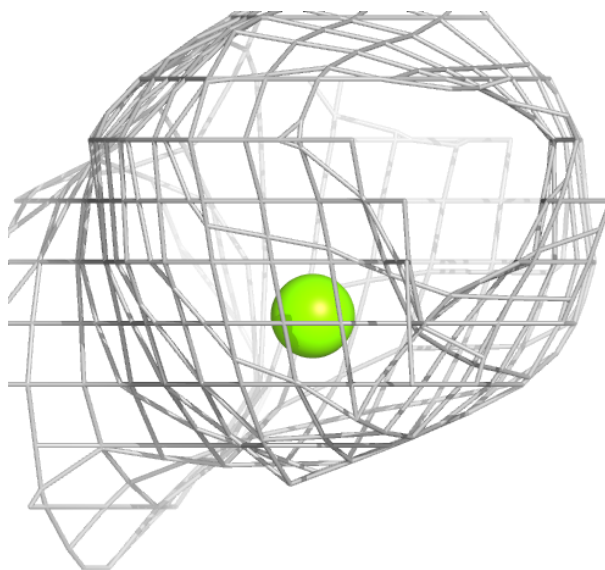
Electron density around MG b 603:

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



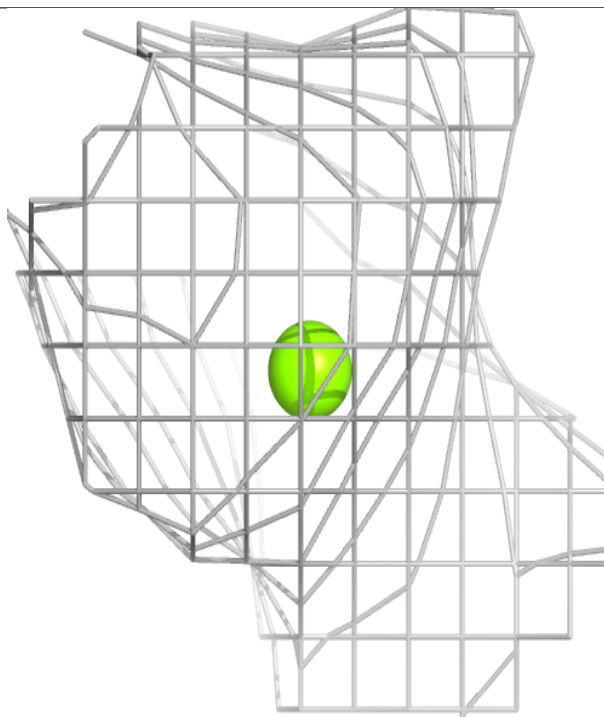
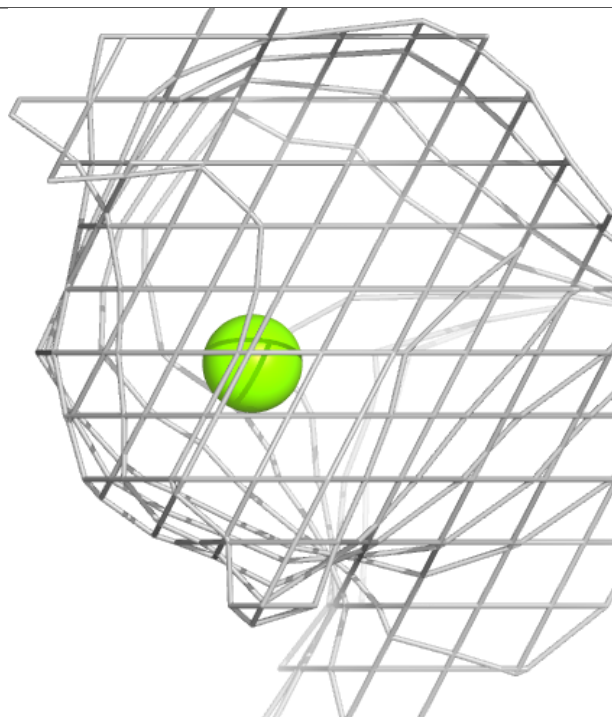
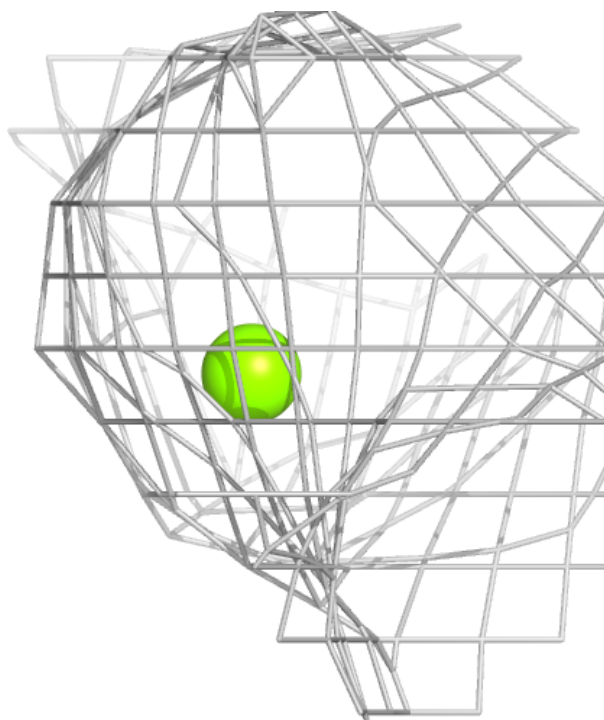
Electron density around MG U 605:

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



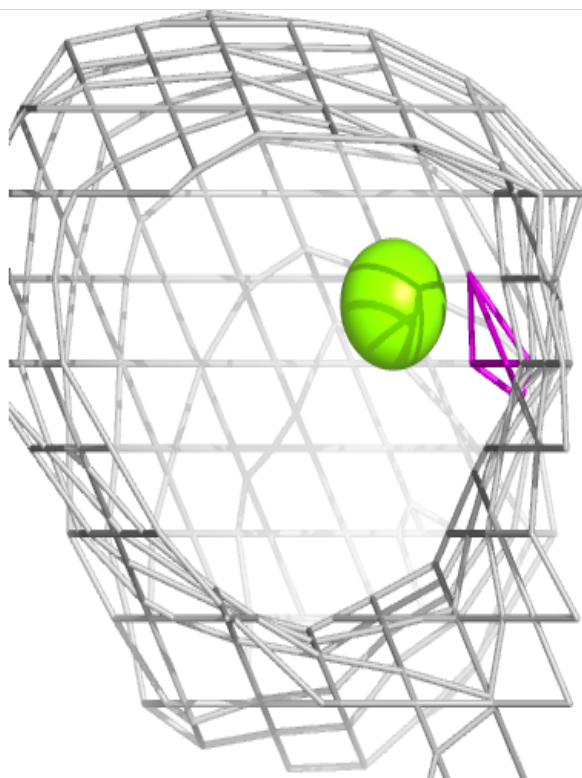
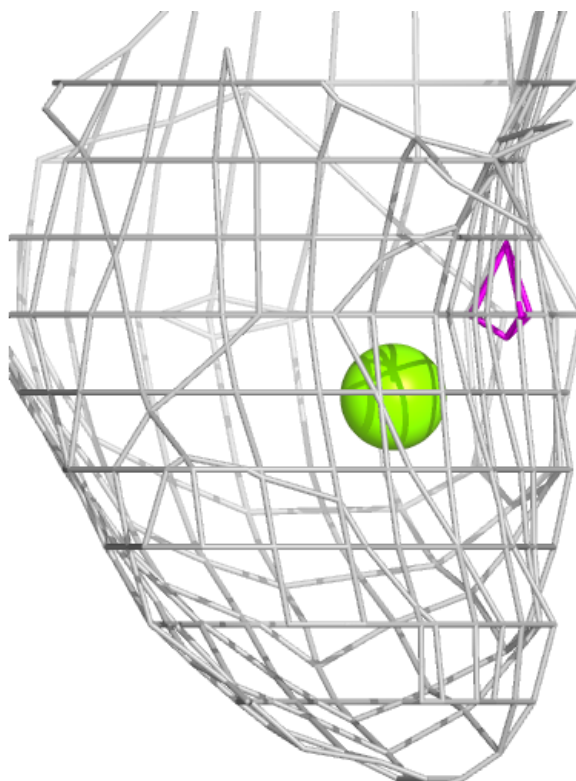
Electron density around MG D 606:

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



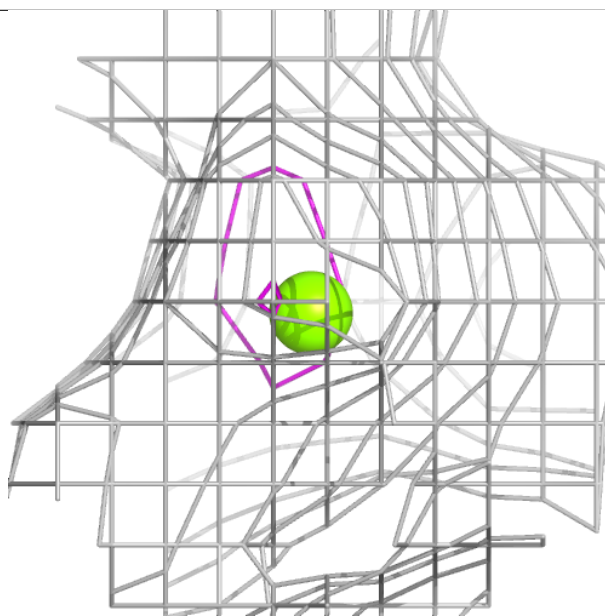
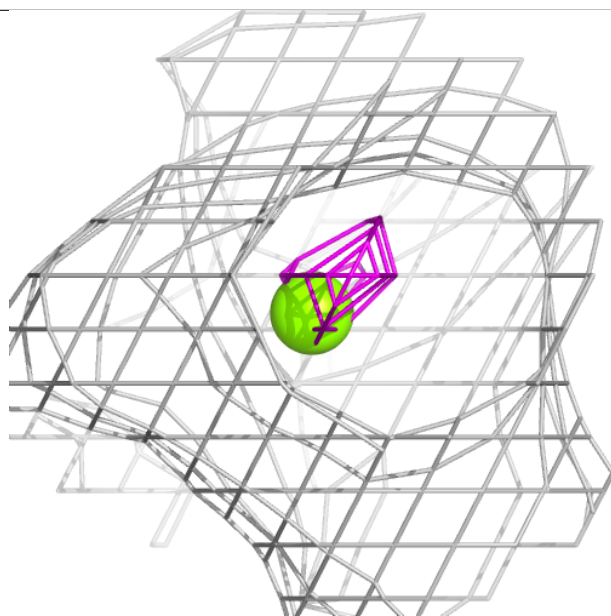
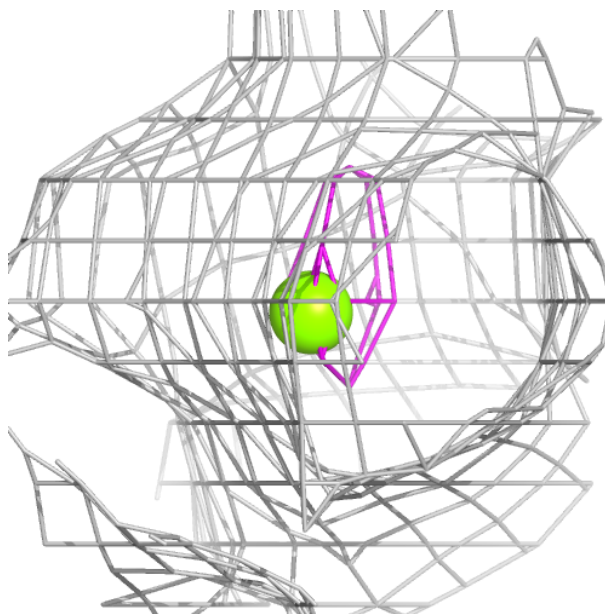
Electron density around MG E 607:

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



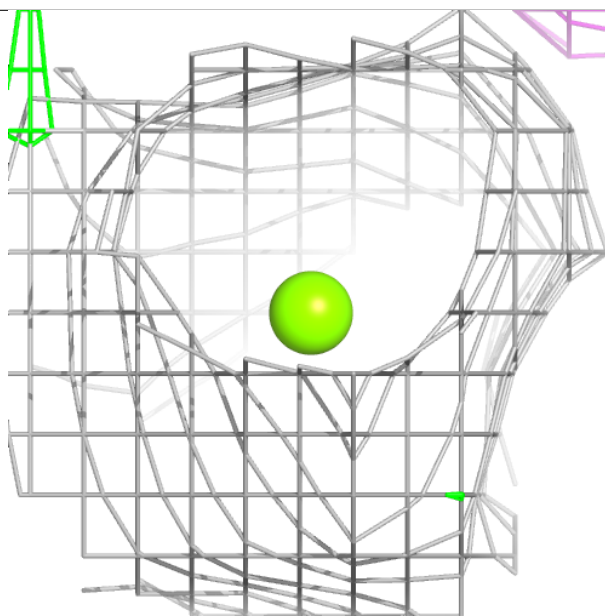
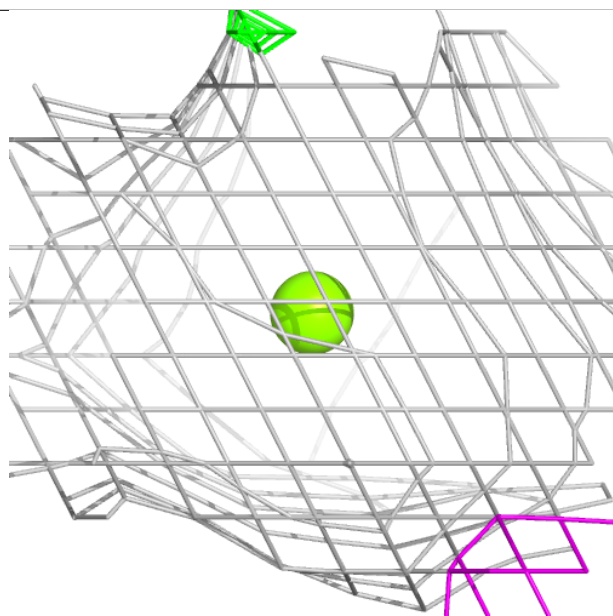
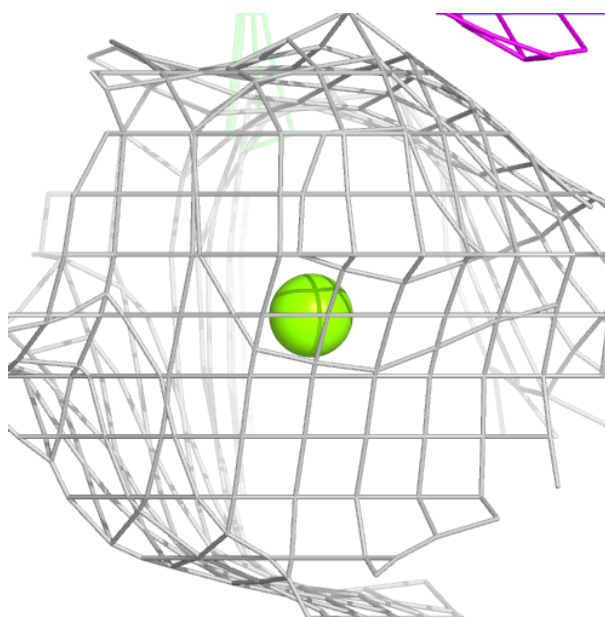
Electron density around MG H 603:

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



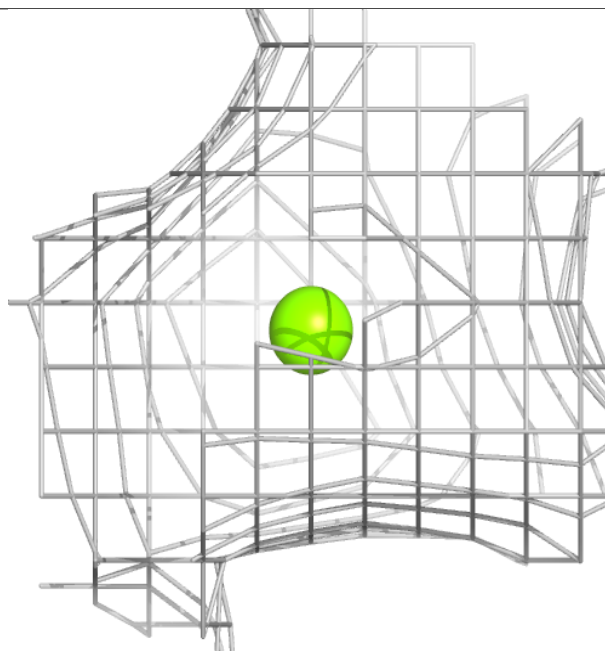
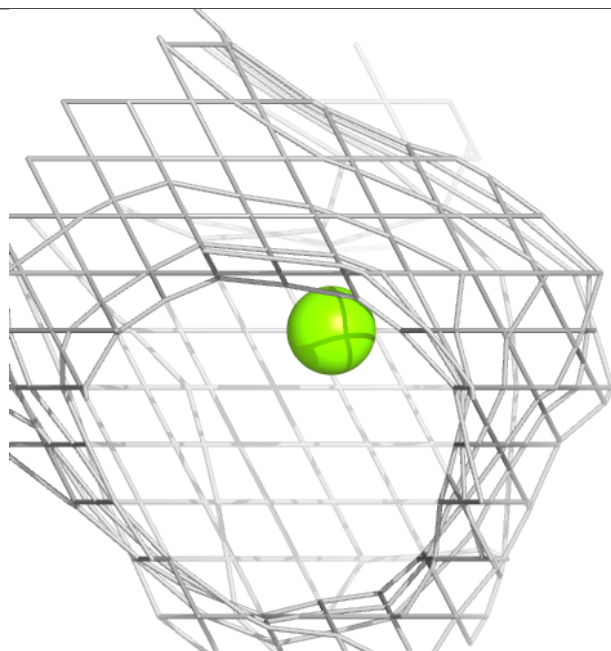
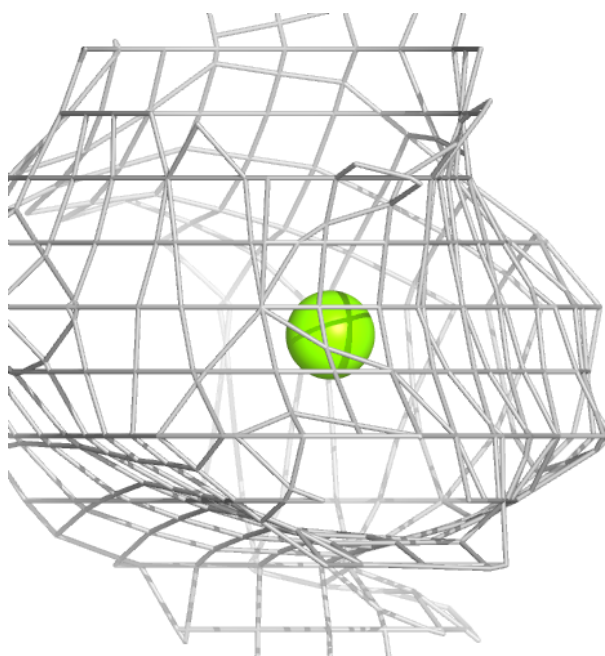
Electron density around MG M 603:

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



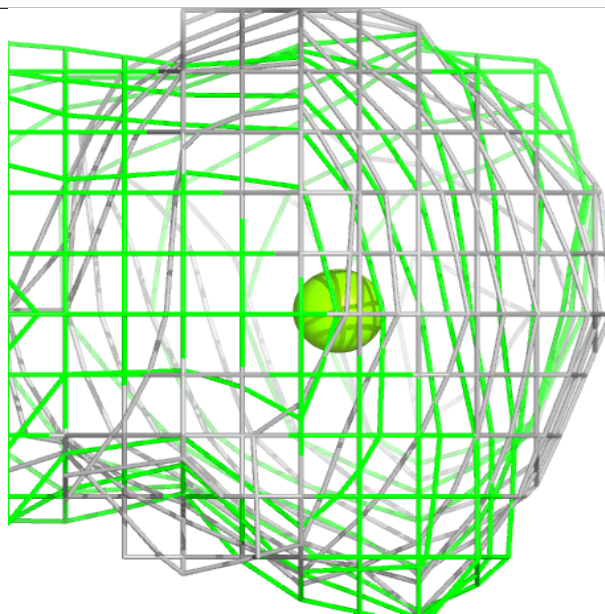
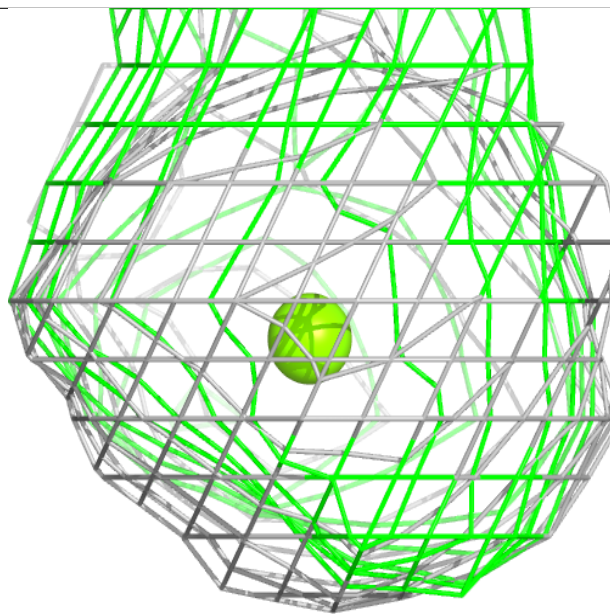
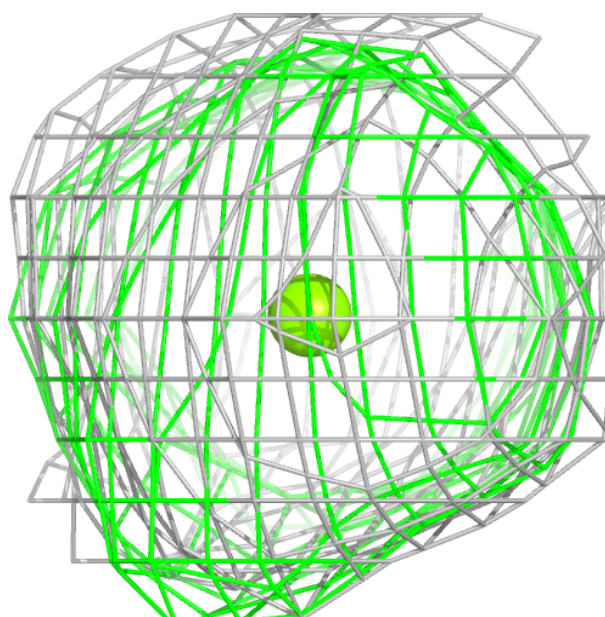
Electron density around MG V 604:

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



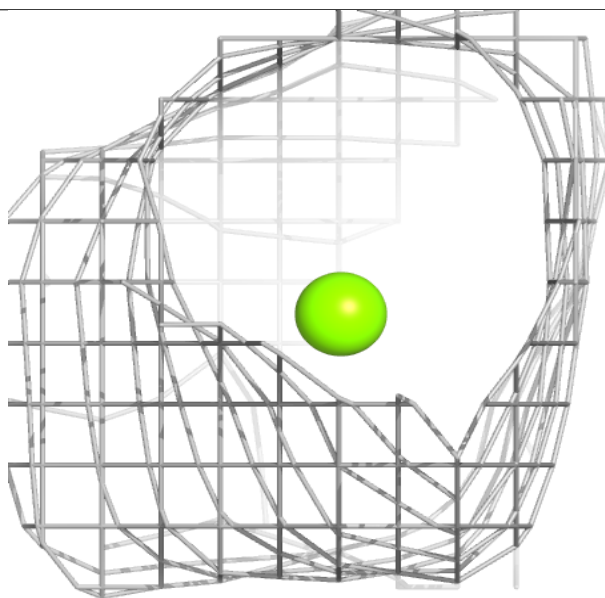
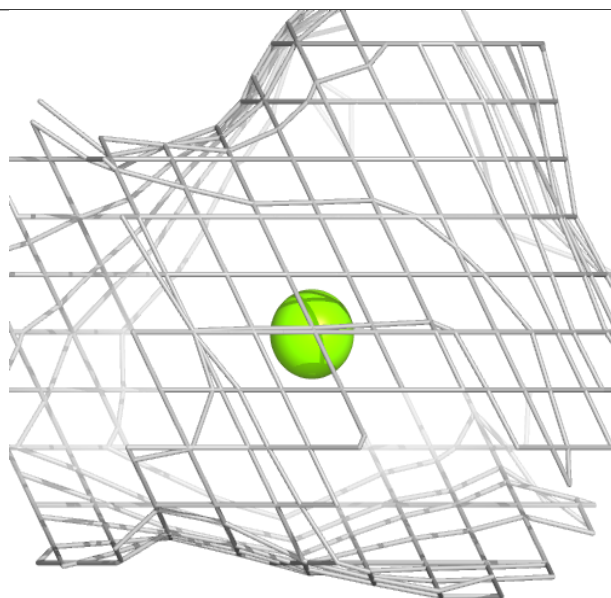
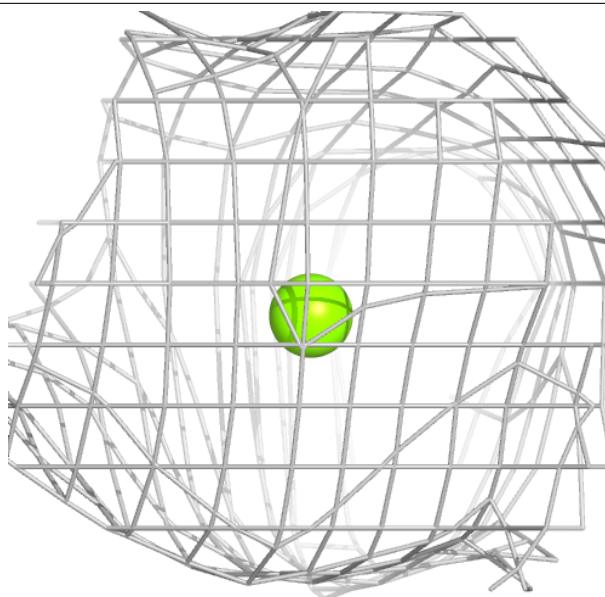
Electron density around MG H 604:

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



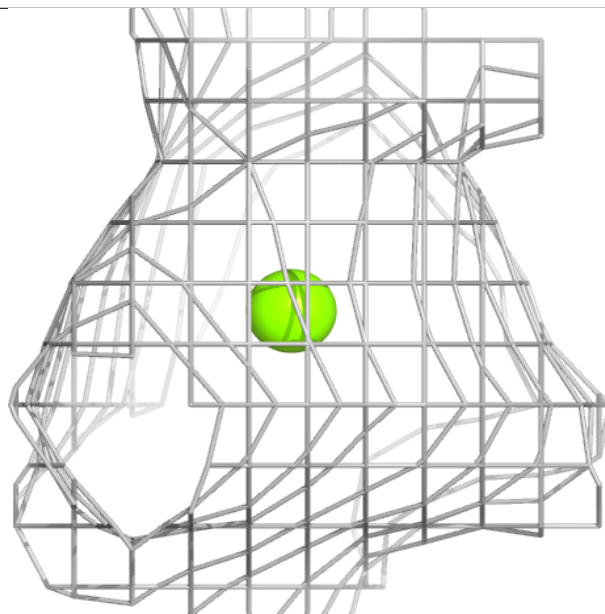
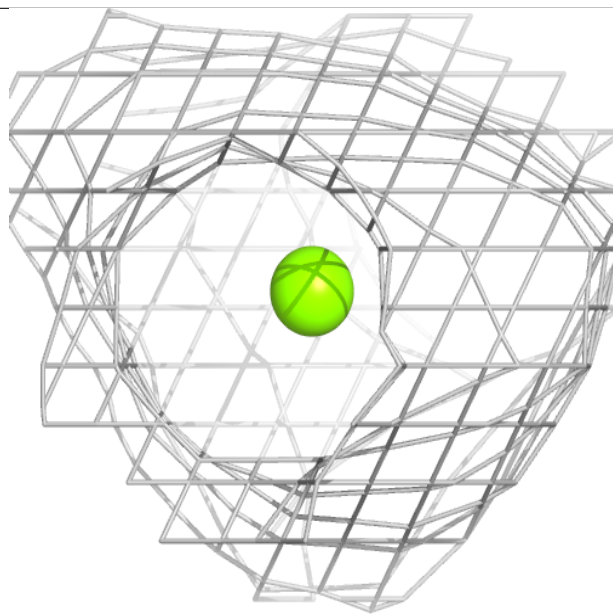
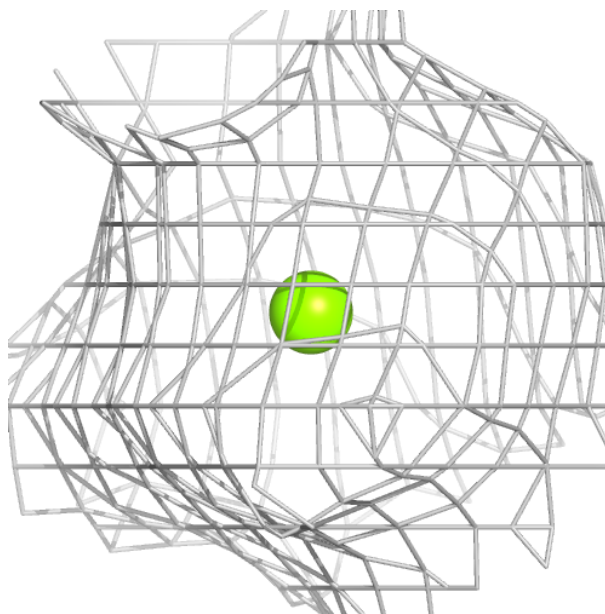
Electron density around MG F 604:

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



Electron density around MG A 604:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.