



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:33 PM UTC

PDB ID : 6KXU / pdb_00006kxu
Title : BON1
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Deposited on : 2019-09-12
Resolution : 2.83 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

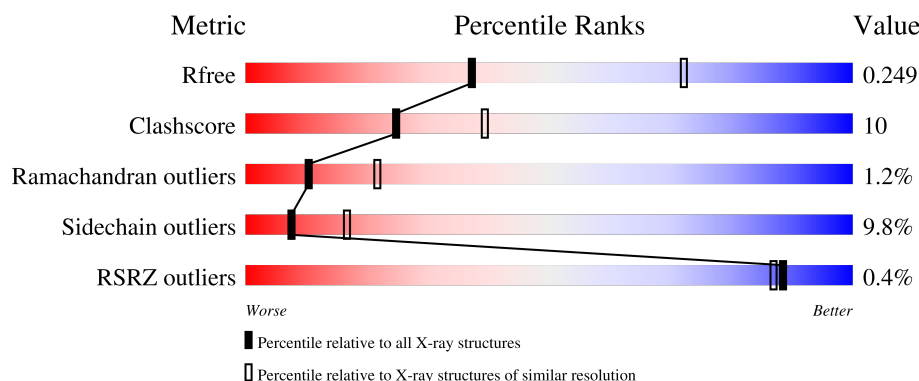
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	553	75% 21% • •
1	C	553	74% 22% •
1	D	553	% 72% 24% • •
1	F	553	% 74% 22% •
2	B	528	70% 22% • • 5%

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Mol	Chain	Length	Quality of chain
3	E	548	73% 21%
4	G	526	2% 70% 23%
5	H	553	74% 20%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 33483 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 Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4242	2699	711	819	13			
1	C	553	Total	C	N	O	S	0	0	0
			4299	2735	719	832	13			
1	D	553	Total	C	N	O	S	0	0	0
			4299	2735	719	832	13			
1	F	553	Total	C	N	O	S	0	0	0
			4299	2735	719	832	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q941L3
A	-8	THR	-	expression tag	UNP Q941L3
A	-7	SER	-	expression tag	UNP Q941L3
A	-6	SER	-	expression tag	UNP Q941L3
A	-5	MET	-	expression tag	UNP Q941L3
A	-4	ALA	-	expression tag	UNP Q941L3
A	-3	ASP	-	expression tag	UNP Q941L3
A	-2	ILE	-	expression tag	UNP Q941L3
A	-1	GLY	-	expression tag	UNP Q941L3
A	0	SER	-	expression tag	UNP Q941L3
C	-9	GLY	-	expression tag	UNP Q941L3
C	-8	THR	-	expression tag	UNP Q941L3
C	-7	SER	-	expression tag	UNP Q941L3
C	-6	SER	-	expression tag	UNP Q941L3
C	-5	MET	-	expression tag	UNP Q941L3
C	-4	ALA	-	expression tag	UNP Q941L3
C	-3	ASP	-	expression tag	UNP Q941L3
C	-2	ILE	-	expression tag	UNP Q941L3
C	-1	GLY	-	expression tag	UNP Q941L3
C	0	SER	-	expression tag	UNP Q941L3
D	-9	GLY	-	expression tag	UNP Q941L3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	THR	-	expression tag	UNP Q941L3
D	-7	SER	-	expression tag	UNP Q941L3
D	-6	SER	-	expression tag	UNP Q941L3
D	-5	MET	-	expression tag	UNP Q941L3
D	-4	ALA	-	expression tag	UNP Q941L3
D	-3	ASP	-	expression tag	UNP Q941L3
D	-2	ILE	-	expression tag	UNP Q941L3
D	-1	GLY	-	expression tag	UNP Q941L3
D	0	SER	-	expression tag	UNP Q941L3
F	-9	GLY	-	expression tag	UNP Q941L3
F	-8	THR	-	expression tag	UNP Q941L3
F	-7	SER	-	expression tag	UNP Q941L3
F	-6	SER	-	expression tag	UNP Q941L3
F	-5	MET	-	expression tag	UNP Q941L3
F	-4	ALA	-	expression tag	UNP Q941L3
F	-3	ASP	-	expression tag	UNP Q941L3
F	-2	ILE	-	expression tag	UNP Q941L3
F	-1	GLY	-	expression tag	UNP Q941L3
F	0	SER	-	expression tag	UNP Q941L3

- Molecule 2 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3932	2507	660	753	12			

- Molecule 3 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	534	Total	C	N	O	S	0	0	0
			4158	2648	696	802	12			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	ALA	-	expression tag	UNP Q941L3
E	-3	ASP	-	expression tag	UNP Q941L3
E	-2	ILE	-	expression tag	UNP Q941L3
E	-1	GLY	-	expression tag	UNP Q941L3
E	0	SER	-	expression tag	UNP Q941L3

- Molecule 4 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	504	Total	C	N	O	S	0	0	0
			3930	2503	661	754	12			

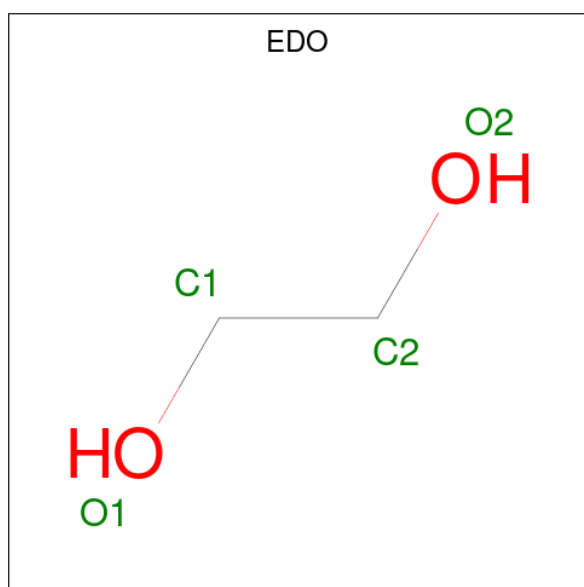
- Molecule 5 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	543	Total	C	N	O	S	0	0	0
			4227	2691	706	817	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	GLY	-	expression tag	UNP Q941L3
H	-8	THR	-	expression tag	UNP Q941L3
H	-7	SER	-	expression tag	UNP Q941L3
H	-6	SER	-	expression tag	UNP Q941L3
H	-5	MET	-	expression tag	UNP Q941L3
H	-4	ALA	-	expression tag	UNP Q941L3
H	-3	ASP	-	expression tag	UNP Q941L3
H	-2	ILE	-	expression tag	UNP Q941L3
H	-1	GLY	-	expression tag	UNP Q941L3
H	0	THR	-	expression tag	UNP Q941L3

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total 1	Cl 1	0	0
9	D	1	Total 1	Cl 1	0	0

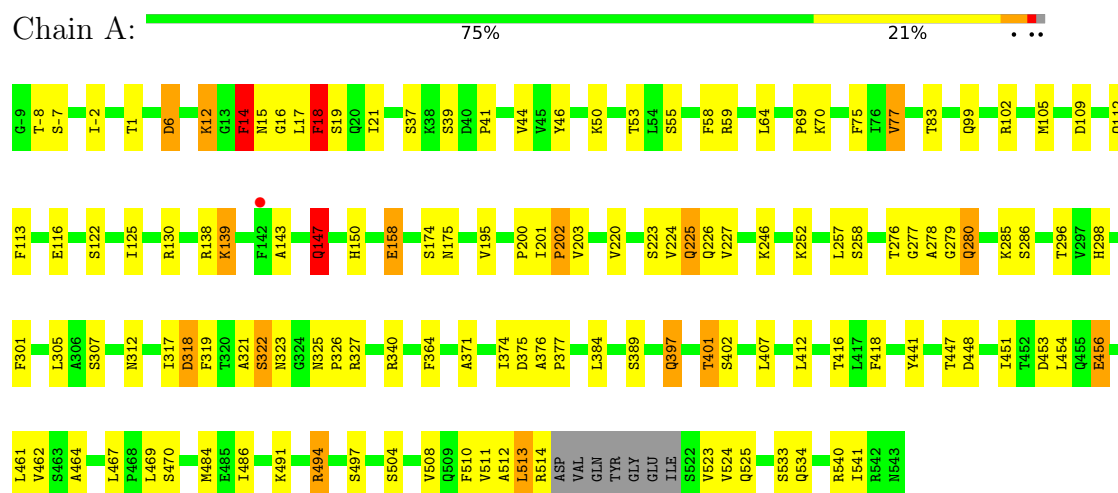
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total 4	O 4	0	0
10	B	6	Total 6	O 6	0	0
10	C	7	Total 7	O 7	0	0
10	D	3	Total 3	O 3	0	0
10	E	1	Total 1	O 1	0	0
10	H	2	Total 2	O 2	0	0

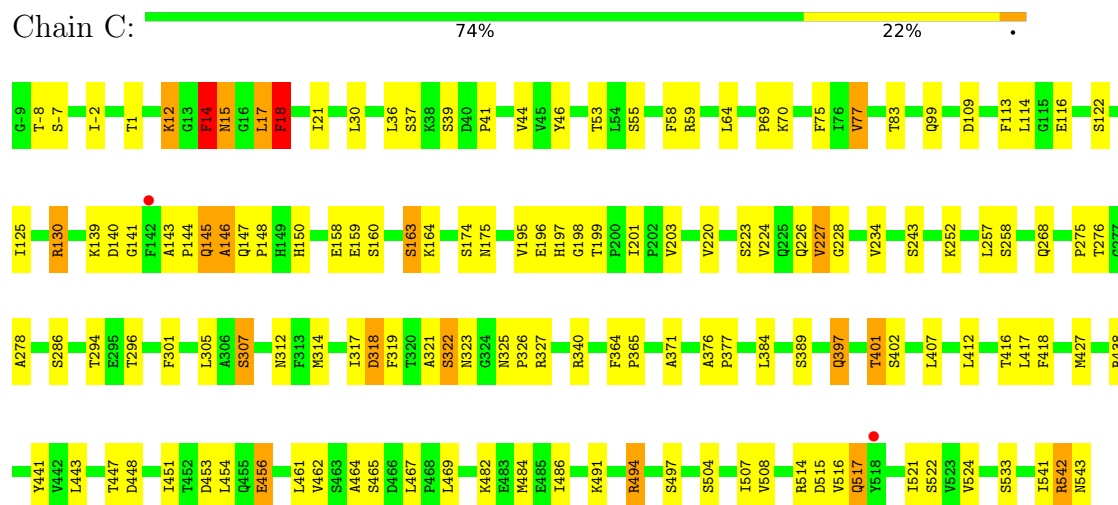
3 Residue-property plots

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

• Molecule 1: Protein BONZAI 1

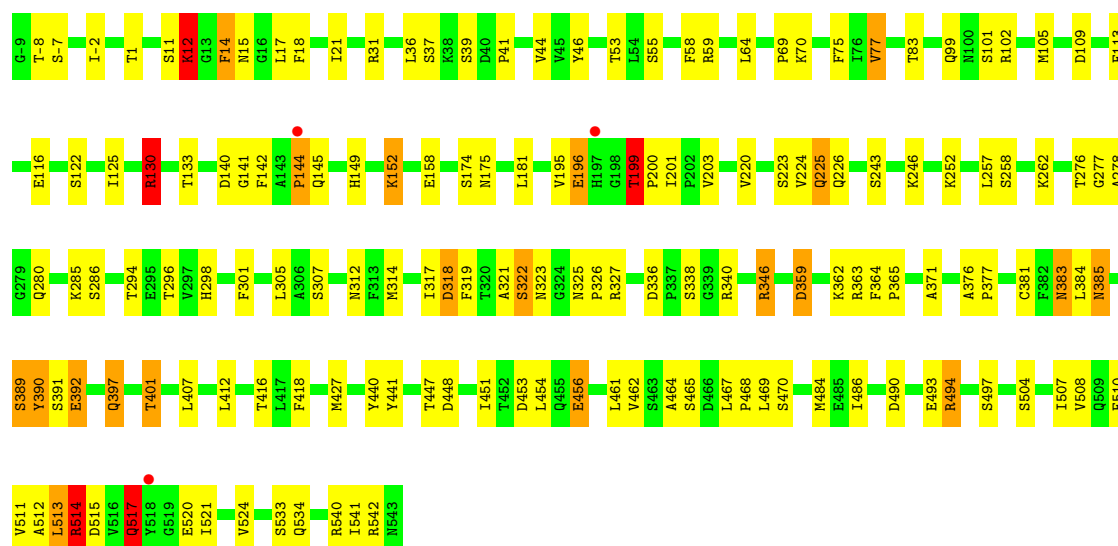


• Molecule 1: Protein BONZAI 1

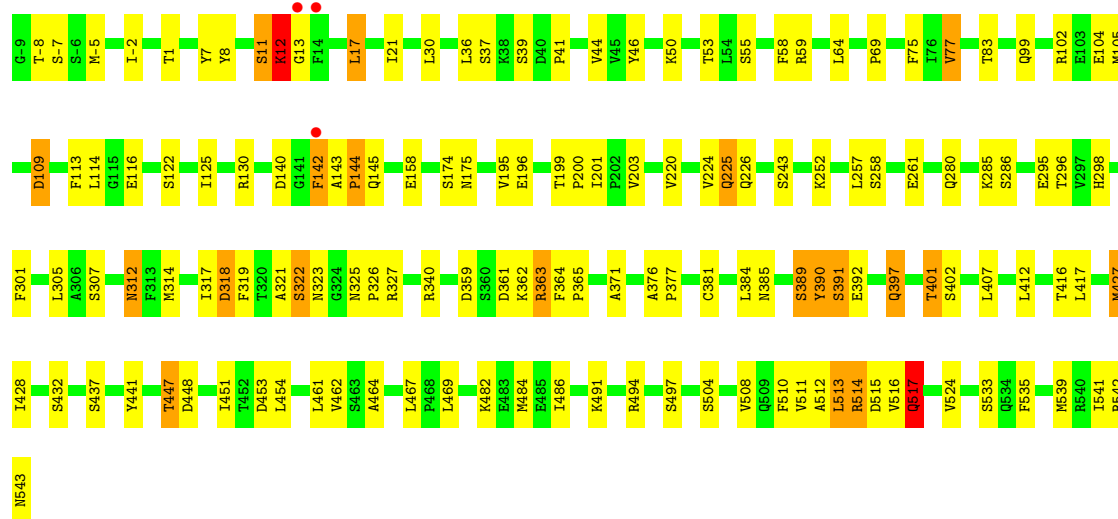
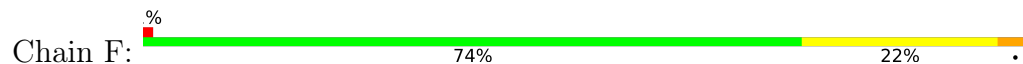


• Molecule 1: Protein BONZAI 1

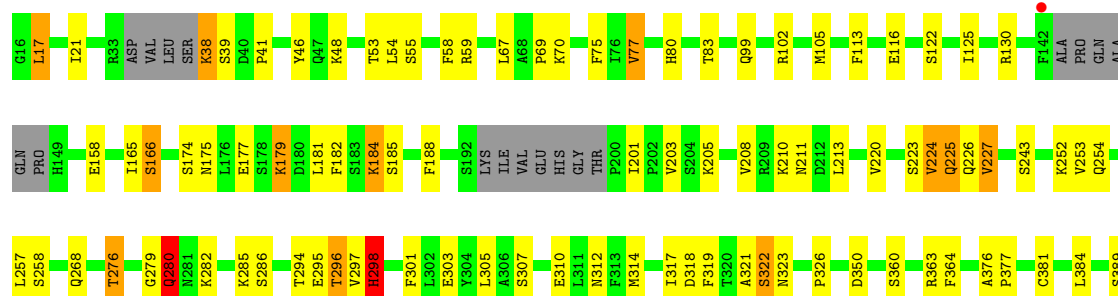


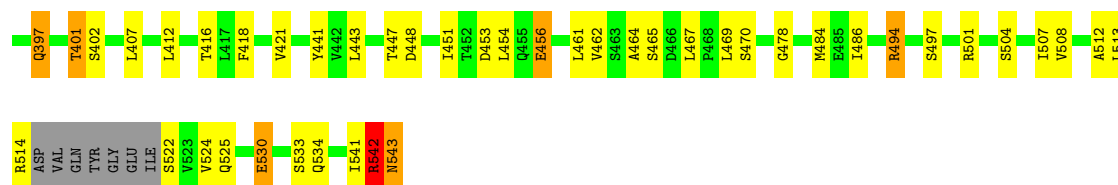


• Molecule 1: Protein BONZAI 1



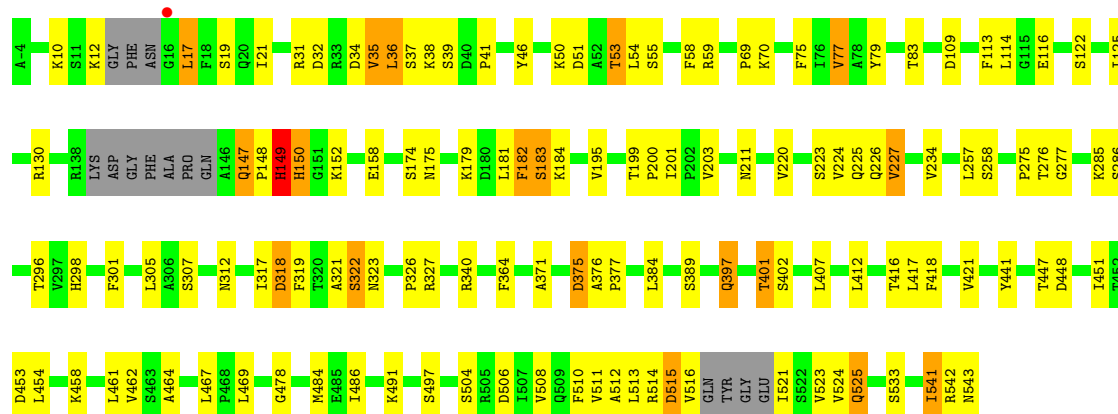
• Molecule 2: Protein BONZAI 1





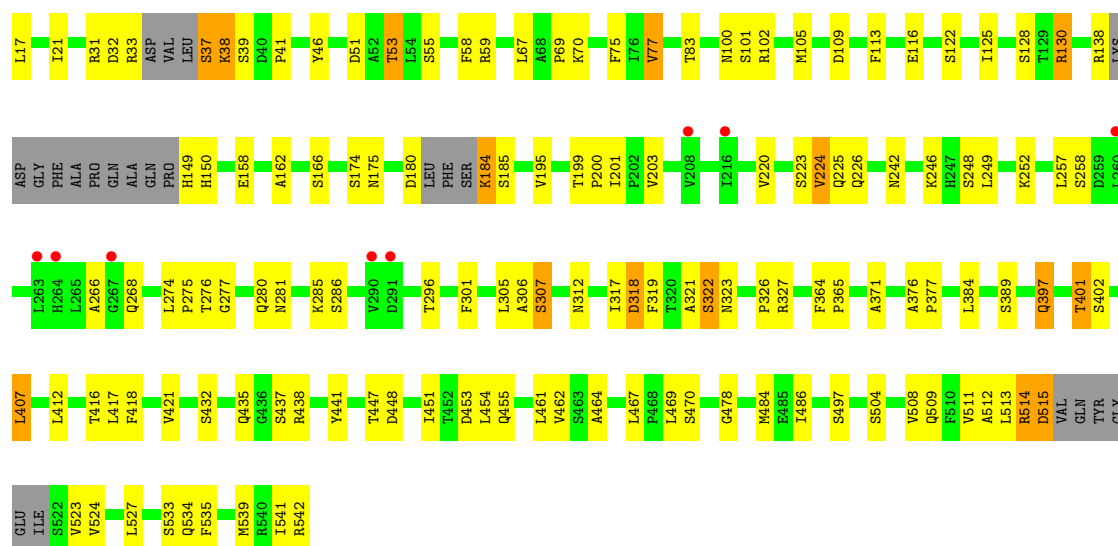
• Molecule 3: Protein BONZAI 1

Chain E: 73% 21%



• Molecule 4: Protein BONZAI 1

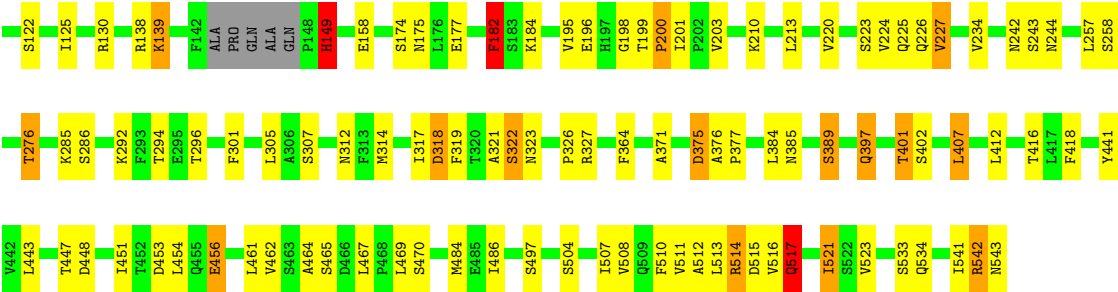
Chain G: 70% 23%



• Molecule 5: Protein BONZAI 1

Chain H: 74% 20%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.41Å 118.70Å 222.32Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	82.31 – 2.83 82.31 – 2.83	Depositor EDS
% Data completeness (in resolution range)	98.2 (82.31-2.83) 98.2 (82.31-2.83)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.204 , 0.249 0.203 , 0.249	Depositor DCC
R_{free} test set	7470 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	69.9	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.246 for h,-k,-l	Xtriage
Reported twinning fraction	0.733 for H, K, L 0.267 for -h,-k,l	Depositor
Outliers	7 of 148582 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33483	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1000e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, GOL, MN, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.55	0/4323	1.07	10/5847 (0.2%)
1	C	0.57	1/4382 (0.0%)	1.08	5/5929 (0.1%)
1	D	0.58	1/4382 (0.0%)	1.13	20/5929 (0.3%)
1	F	0.56	1/4382 (0.0%)	1.09	9/5929 (0.2%)
2	B	0.56	1/4004 (0.0%)	1.11	15/5408 (0.3%)
3	E	0.54	0/4234	1.08	10/5726 (0.2%)
4	G	0.56	0/4001	1.06	8/5408 (0.1%)
5	H	0.55	0/4305	1.09	11/5818 (0.2%)
All	All	0.56	4/34013 (0.0%)	1.09	88/45994 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	F	0	1
2	B	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	HIS	CE1-NE2	7.71	1.40	1.32
1	F	447	THR	CB-OG1	6.17	1.53	1.43
2	B	80	HIS	CE1-NE2	6.10	1.38	1.32
1	D	392	GLU	CD-OE2	5.15	1.35	1.25

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	447	THR	CA-CB-OG1	14.00	130.59	109.60
2	B	38	LYS	CB-CA-C	11.43	131.82	110.10
1	F	447	THR	N-CA-CB	11.04	129.75	111.31
1	D	298	HIS	CB-CA-C	9.25	125.16	109.53
1	C	416	THR	CA-CB-OG1	9.10	123.25	109.60
1	F	416	THR	CA-CB-OG1	9.06	123.19	109.60
2	B	298	HIS	CB-CA-C	8.83	124.46	109.53
3	E	416	THR	CA-CB-OG1	8.81	122.82	109.60
5	H	416	THR	CA-CB-OG1	8.70	122.65	109.60
2	B	416	THR	CA-CB-OG1	8.67	122.61	109.60
1	A	416	THR	CA-CB-OG1	8.67	122.60	109.60
4	G	416	THR	CA-CB-OG1	8.61	122.52	109.60
1	D	383	ASN	CA-CB-CG	8.39	120.99	112.60
1	A	540	ARG	CG-CD-NE	-8.39	93.54	112.00
1	D	416	THR	CA-CB-OG1	8.36	122.15	109.60
1	C	494	ARG	CB-CG-CD	8.27	130.32	111.30
2	B	279	GLY	CA-C-N	8.06	136.93	121.54
2	B	279	GLY	C-N-CA	8.06	136.93	121.54
1	A	540	ARG	CB-CG-CD	7.93	129.55	111.30
5	H	182	PHE	CA-CB-CG	7.90	121.70	113.80
1	D	276	THR	CB-CA-C	7.69	124.07	109.37
1	A	18	PHE	CB-CA-C	7.68	121.78	110.26
1	D	494	ARG	CB-CG-CD	7.65	128.89	111.30
5	H	200	PRO	CB-CA-C	-7.64	98.95	111.56
1	D	540	ARG	CG-CD-NE	-7.59	95.29	112.00
4	G	130	ARG	CB-CG-CD	7.58	128.75	111.30
1	A	494	ARG	CB-CG-CD	7.46	128.46	111.30
1	F	109	ASP	CA-CB-CG	7.18	119.78	112.60
1	D	364	PHE	CB-CA-C	-6.95	102.15	110.15
2	B	280	GLN	CB-CA-C	6.91	124.17	110.42
1	F	361	ASP	CA-CB-CG	6.85	119.45	112.60
1	D	514	ARG	CB-CA-C	-6.69	97.10	110.42
5	H	364	PHE	CB-CA-C	-6.49	102.69	110.15
2	B	530	GLU	CB-CG-CD	-6.18	102.09	112.60
2	B	179	LYS	CA-CB-CG	6.18	126.46	114.10
2	B	276	THR	CB-CA-C	6.17	120.83	111.70
1	F	364	PHE	CB-CA-C	-6.16	103.07	110.15
5	H	149	HIS	CB-CA-C	6.14	121.73	111.30
3	E	364	PHE	CB-CA-C	-6.13	103.10	110.15
1	A	364	PHE	CB-CA-C	-6.12	103.11	110.15
3	E	150	HIS	N-CA-CB	6.11	120.81	110.49
4	G	364	PHE	CB-CA-C	-6.08	103.16	110.15
5	H	521	ILE	N-CA-CB	6.07	117.47	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	298	HIS	CB-CA-C	5.97	119.63	109.53
2	B	364	PHE	CB-CA-C	-5.95	103.31	110.15
1	C	364	PHE	CB-CA-C	-5.90	103.36	110.15
1	F	140	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	225	GLN	CB-CG-CD	-5.87	102.62	112.60
4	G	421	VAL	N-CA-CB	5.82	117.36	110.55
4	G	53	THR	CB-CA-C	5.74	121.19	109.76
4	G	150	HIS	CB-CA-C	5.64	120.34	110.64
2	B	363	ARG	CB-CG-CD	5.62	124.23	111.30
2	B	421	VAL	N-CA-CB	5.56	117.05	110.55
4	G	416	THR	CB-CA-C	5.55	120.05	110.77
1	D	346	ARG	CB-CG-CD	5.54	124.05	111.30
1	D	340	ARG	CG-CD-NE	-5.54	99.81	112.00
5	H	276	THR	CB-CA-C	5.53	119.98	111.85
3	E	53	THR	CB-CA-C	5.53	120.76	109.76
1	F	416	THR	CB-CA-C	5.52	120.00	110.77
1	A	416	THR	CB-CA-C	5.50	119.95	110.77
2	B	416	THR	CB-CA-C	5.49	119.94	110.77
3	E	506	ASP	CA-CB-CG	5.48	118.08	112.60
5	H	416	THR	CB-CA-C	5.48	119.92	110.77
2	B	177	GLU	CB-CG-CD	-5.47	103.30	112.60
5	H	54	LEU	N-CA-CB	-5.46	102.00	110.57
2	B	542	ARG	CB-CG-CD	5.45	123.84	111.30
5	H	53	THR	CB-CA-C	5.39	120.49	109.76
1	C	416	THR	CB-CA-C	5.38	119.75	110.77
1	D	130	ARG	CG-CD-NE	5.33	123.73	112.00
1	D	196	GLU	CB-CG-CD	5.32	121.64	112.60
1	D	18	PHE	CB-CA-C	5.29	117.78	110.16
1	D	416	THR	CB-CA-C	5.28	119.59	110.77
5	H	31	ARG	CB-CA-C	5.27	120.12	111.74
3	E	149	HIS	CA-C-N	5.27	131.60	121.54
3	E	149	HIS	C-N-CA	5.27	131.60	121.54
3	E	416	THR	CB-CA-C	5.26	119.55	110.77
1	D	298	HIS	N-CA-CB	5.24	117.97	110.06
1	A	147	GLN	CB-CA-C	5.18	117.80	109.51
1	C	14	PHE	CB-CA-C	5.13	118.50	110.19
1	D	199	THR	CA-CB-OG1	5.13	117.30	109.60
1	A	14	PHE	CA-CB-CG	5.10	118.90	113.80
3	E	149	HIS	N-CA-C	5.08	121.63	110.80
4	G	365	PRO	CB-CA-C	-5.06	105.27	111.64
3	E	421	VAL	N-CA-CB	5.02	117.00	110.57
1	D	199	THR	CB-CA-C	5.02	117.50	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	490	ASP	CB-CA-C	5.02	118.73	110.95
1	D	133	THR	CA-CB-OG1	-5.02	102.07	109.60
1	A	6	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	PHE	Peptide
2	B	184	LYS	Peptide
2	B	296	THR	Peptide
1	D	12	LYS	Peptide
1	F	11	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4242	0	4246	79	0
1	C	4299	0	4297	81	0
1	D	4299	0	4298	93	0
1	F	4299	0	4295	101	0
2	B	3932	0	3944	77	0
3	E	4158	0	4172	76	0
4	G	3930	0	3945	90	0
5	H	4227	0	4233	82	0
6	A	12	0	18	0	0
6	B	4	0	6	0	0
6	C	16	0	24	0	0
6	D	4	0	6	1	0
6	F	8	0	12	0	0
6	G	4	0	6	1	0
6	H	8	0	12	0	0
7	A	6	0	8	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	2	0	0	0	0
8	E	1	0	0	0	0
8	F	2	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	4	0	0	0	0
10	B	6	0	0	0	0
10	C	7	0	0	1	0
10	D	3	0	0	0	0
10	E	1	0	0	0	0
10	H	2	0	0	1	0
All	All	33483	0	33522	655	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 10.

All (655) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:427:MET:HG3	4:G:184:LYS:N	1.61	1.15
1:F:318:ASP:OD2	1:F:447:THR:OG1	1.65	1.14
1:F:142:PHE:O	1:F:144:PRO:HD3	1.49	1.12
5:H:102:ARG:NH2	10:H:701:HOH:O	1.90	1.02
1:C:195:VAL:CG2	1:C:198:GLY:O	2.16	0.94
1:F:12:LYS:NZ	1:F:17:LEU:HD11	1.84	0.92
2:B:319:PHE:HE1	2:B:407:LEU:HD23	1.34	0.91
1:D:389:SER:O	1:D:390:TYR:O	1.89	0.90
4:G:274:LEU:O	4:G:281:ASN:HB3	1.71	0.89
1:A:277:GLY:O	1:A:279:GLY:N	2.05	0.89
1:A:16:GLY:O	1:A:225:GLN:CG	2.21	0.89
1:F:385:ASN:HD21	1:F:391:SER:HB3	1.38	0.88
1:F:427:MET:CG	4:G:184:LYS:N	2.36	0.88
4:G:162:ALA:O	4:G:224:VAL:HG21	1.75	0.87
1:A:16:GLY:O	1:A:225:GLN:HG2	1.75	0.87
1:D:383:ASN:HB3	1:D:385:ASN:ND2	1.91	0.86
1:C:195:VAL:HG23	1:C:198:GLY:O	1.75	0.86
3:E:275:PRO:O	3:E:277:GLY:N	2.09	0.85
1:D:285:LYS:HE2	5:H:389:SER:HB2	1.58	0.84
1:A:143:ALA:O	1:A:147:GLN:HB3	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ASP:HB3	2:B:524:VAL:HG21	1.59	0.83
3:E:10:LYS:HD3	3:E:541:ILE:HD11	1.59	0.82
2:B:213:LEU:HD21	1:D:427:MET:HE3	1.59	0.82
2:B:297:VAL:HB	1:F:295:GLU:HB2	1.62	0.82
1:F:389:SER:O	1:F:390:TYR:O	1.98	0.81
1:D:389:SER:O	1:D:390:TYR:C	2.23	0.81
4:G:249:LEU:CD1	4:G:274:LEU:HD22	2.12	0.80
2:B:166:SER:HB3	2:B:298:HIS:HB3	1.63	0.80
1:F:318:ASP:CB	1:F:447:THR:HB	2.12	0.79
1:F:12:LYS:HZ2	1:F:17:LEU:HD11	1.45	0.78
2:B:319:PHE:CE1	2:B:407:LEU:HD23	2.19	0.77
1:D:17:LEU:HA	1:D:225:GLN:NE2	1.99	0.77
1:F:389:SER:O	1:F:390:TYR:C	2.27	0.77
4:G:31:ARG:HB3	4:G:67:LEU:CD2	2.16	0.75
4:G:17:LEU:O	6:G:601:EDO:H21	1.86	0.75
4:G:249:LEU:HD13	4:G:274:LEU:CD2	2.17	0.75
5:H:542:ARG:O	5:H:543:ASN:HB2	1.87	0.75
3:E:184:LYS:HD2	3:E:211:ASN:OD1	1.86	0.75
4:G:249:LEU:CD1	4:G:274:LEU:CD2	2.64	0.75
2:B:317:ILE:HD12	2:B:384:LEU:HD11	1.69	0.75
3:E:317:ILE:HD12	3:E:384:LEU:HD11	1.69	0.74
3:E:17:LEU:HD12	3:E:19:SER:OG	1.88	0.74
3:E:147:GLN:HG3	3:E:148:PRO:HD2	1.69	0.74
1:C:307:SER:O	1:C:438:ARG:NH2	2.16	0.72
3:E:21:ILE:HD13	3:E:125:ILE:HG21	1.70	0.72
5:H:317:ILE:HD12	5:H:384:LEU:HD11	1.71	0.72
2:B:478:GLY:HA2	2:B:514:ARG:HH21	1.52	0.72
1:D:102:ARG:HH22	1:D:105:MET:HE3	1.55	0.71
1:D:317:ILE:HD12	1:D:384:LEU:HD11	1.72	0.71
4:G:317:ILE:HD12	4:G:384:LEU:HD11	1.71	0.71
1:F:318:ASP:HB2	1:F:447:THR:HB	1.72	0.71
1:F:317:ILE:HD12	1:F:384:LEU:HD11	1.73	0.70
1:C:317:ILE:HD12	1:C:384:LEU:HD11	1.73	0.70
3:E:17:LEU:HD11	3:E:79:TYR:CD2	2.26	0.70
4:G:478:GLY:HA2	4:G:514:ARG:HH21	1.56	0.70
1:D:517:GLN:HG2	1:D:520:GLU:HB2	1.72	0.69
2:B:542:ARG:HG3	2:B:543:ASN:N	2.08	0.69
1:F:11:SER:O	1:F:12:LYS:HB2	1.92	0.69
1:D:363:ARG:HB3	1:D:392:GLU:HB3	1.75	0.69
1:F:359:ASP:O	1:F:362:LYS:HD3	1.93	0.68
1:C:453:ASP:HB2	1:C:456:GLU:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:ARG:HG2	1:C:543:ASN:H	1.57	0.68
1:F:516:VAL:O	1:F:517:GLN:HB2	1.92	0.68
1:C:17:LEU:O	1:C:18:PHE:O	2.11	0.68
1:D:383:ASN:HB3	1:D:385:ASN:HD21	1.59	0.68
1:D:453:ASP:HB2	1:D:456:GLU:HG2	1.76	0.68
1:C:199:THR:HG23	5:H:210:LYS:CE	2.23	0.68
2:B:38:LYS:HB3	2:B:67:LEU:HD21	1.76	0.67
1:A:317:ILE:HD12	1:A:384:LEU:HD11	1.75	0.67
1:C:21:ILE:HD13	1:C:125:ILE:HG21	1.77	0.67
1:A:453:ASP:HB2	1:A:456:GLU:HG2	1.76	0.67
1:F:21:ILE:HD13	1:F:125:ILE:HG21	1.76	0.67
1:A:21:ILE:HD13	1:A:125:ILE:HG21	1.75	0.67
1:D:31:ARG:HH12	6:D:601:EDO:H12	1.59	0.67
4:G:249:LEU:HD13	4:G:274:LEU:HD22	1.76	0.67
4:G:21:ILE:HD13	4:G:125:ILE:HG21	1.76	0.67
5:H:453:ASP:HB2	5:H:456:GLU:HG2	1.75	0.67
2:B:453:ASP:HB2	2:B:456:GLU:HG2	1.77	0.66
1:C:203:VAL:CG1	1:C:226:GLN:HB3	2.24	0.66
1:A:203:VAL:CG1	1:A:226:GLN:HB3	2.25	0.66
1:F:514:ARG:CG	1:F:515:ASP:H	2.07	0.66
3:E:17:LEU:HD11	3:E:79:TYR:HD2	1.61	0.66
1:D:17:LEU:HA	1:D:225:GLN:HE22	1.61	0.65
1:F:385:ASN:HD21	1:F:391:SER:CB	2.07	0.65
1:F:203:VAL:CG1	1:F:226:GLN:HB3	2.26	0.65
1:D:21:ILE:HD13	1:D:125:ILE:HG21	1.77	0.65
2:B:21:ILE:HD13	2:B:125:ILE:HG21	1.77	0.65
4:G:203:VAL:CG1	4:G:226:GLN:HB3	2.27	0.65
1:D:203:VAL:CG1	1:D:226:GLN:HB3	2.27	0.64
3:E:17:LEU:HG	3:E:17:LEU:O	1.97	0.64
1:A:470:SER:OG	1:A:534:GLN:NE2	2.31	0.64
2:B:203:VAL:CG1	2:B:226:GLN:HB3	2.28	0.64
1:D:363:ARG:CB	1:D:392:GLU:CD	2.70	0.64
5:H:21:ILE:HD13	5:H:125:ILE:HG21	1.78	0.64
5:H:184:LYS:HE2	5:H:213:LEU:HD11	1.78	0.64
5:H:203:VAL:CG1	5:H:226:GLN:HB3	2.28	0.64
2:B:99:GLN:O	1:F:102:ARG:NH2	2.23	0.64
1:F:12:LYS:NZ	1:F:17:LEU:CD1	2.59	0.64
1:D:363:ARG:HB2	1:D:392:GLU:CD	2.23	0.64
1:D:102:ARG:NH2	1:D:105:MET:HE3	2.13	0.63
1:C:453:ASP:HB2	1:C:456:GLU:CG	2.29	0.63
5:H:17:LEU:HD23	5:H:225:GLN:HE22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:ASP:HB2	1:D:456:GLU:CG	2.29	0.63
1:D:385:ASN:HD22	1:D:385:ASN:H	1.45	0.62
3:E:149:HIS:CE1	3:E:152:LYS:HE3	2.34	0.62
1:C:228:GLY:HA3	10:C:705:HOH:O	1.98	0.62
2:B:213:LEU:CD2	1:D:427:MET:HE3	2.29	0.62
3:E:203:VAL:CG1	3:E:226:GLN:HB3	2.29	0.62
3:E:542:ARG:HG3	3:E:543:ASN:N	2.14	0.62
2:B:310:GLU:OE2	2:B:360:SER:OG	2.12	0.62
1:F:514:ARG:HG3	1:F:515:ASP:H	1.64	0.62
1:F:390:TYR:HE2	1:F:428:ILE:CD1	2.12	0.62
4:G:435:GLN:O	4:G:435:GLN:NE2	2.32	0.62
4:G:435:GLN:O	4:G:435:GLN:CG	2.47	0.61
5:H:453:ASP:HB2	5:H:456:GLU:CG	2.30	0.61
2:B:470:SER:OG	2:B:534:GLN:NE2	2.32	0.61
1:C:203:VAL:HG11	1:C:226:GLN:HB3	1.82	0.61
1:F:12:LYS:HZ2	1:F:17:LEU:CD1	2.14	0.61
1:D:418:PHE:HZ	1:D:447:THR:HG21	1.66	0.61
5:H:29:ASN:HB3	5:H:32:ASP:OD1	2.00	0.61
1:A:453:ASP:HB2	1:A:456:GLU:CG	2.30	0.61
1:A:513:LEU:O	1:A:514:ARG:C	2.44	0.61
1:D:203:VAL:HG11	1:D:226:GLN:HB3	1.82	0.60
4:G:130:ARG:NH1	4:G:158:GLU:OE2	2.34	0.60
4:G:435:GLN:O	4:G:435:GLN:HG3	2.00	0.60
1:D:513:LEU:O	1:D:514:ARG:C	2.44	0.60
5:H:470:SER:OG	5:H:534:GLN:NE2	2.33	0.60
1:A:139:LYS:O	1:A:139:LYS:HG3	2.01	0.60
1:C:17:LEU:HD22	1:C:163:SER:O	2.01	0.60
3:E:542:ARG:HG3	3:E:543:ASN:H	1.66	0.60
4:G:17:LEU:O	4:G:17:LEU:HG	2.01	0.60
4:G:319:PHE:CE2	4:G:407:LEU:HD23	2.35	0.60
1:D:470:SER:OG	1:D:534:GLN:NE2	2.34	0.60
4:G:418:PHE:HZ	4:G:447:THR:HG21	1.66	0.60
5:H:319:PHE:CE2	5:H:407:LEU:HD23	2.36	0.60
1:A:418:PHE:HZ	1:A:447:THR:HG21	1.66	0.60
1:F:130:ARG:NH1	1:F:158:GLU:OE2	2.33	0.60
3:E:35:VAL:O	3:E:37:SER:N	2.34	0.60
3:E:319:PHE:CE2	3:E:407:LEU:HD23	2.37	0.60
5:H:203:VAL:HG11	5:H:226:GLN:HB3	1.82	0.60
2:B:418:PHE:HZ	2:B:447:THR:HG21	1.66	0.60
4:G:470:SER:OG	4:G:534:GLN:NE2	2.33	0.60
1:C:418:PHE:HZ	1:C:447:THR:HG21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:ARG:HG2	1:C:543:ASN:N	2.15	0.60
1:F:175:ASN:O	1:F:286:SER:HB3	2.02	0.60
1:F:319:PHE:CE2	1:F:407:LEU:HD23	2.37	0.59
2:B:453:ASP:HB2	2:B:456:GLU:CG	2.31	0.59
5:H:418:PHE:HZ	5:H:447:THR:HG21	1.66	0.59
2:B:203:VAL:HG11	2:B:226:GLN:HB3	1.84	0.59
5:H:130:ARG:NH1	5:H:158:GLU:OE2	2.33	0.59
2:B:211:ASN:C	1:D:427:MET:HG3	2.28	0.59
1:D:175:ASN:O	1:D:286:SER:HB3	2.03	0.59
3:E:181:LEU:HB3	3:E:183:SER:OG	2.02	0.59
3:E:418:PHE:HZ	3:E:447:THR:HG21	1.66	0.59
1:C:319:PHE:CE2	1:C:407:LEU:HD23	2.37	0.59
3:E:175:ASN:O	3:E:286:SER:HB3	2.03	0.59
3:E:203:VAL:HG11	3:E:226:GLN:HB3	1.83	0.59
5:H:175:ASN:O	5:H:286:SER:HB3	2.03	0.59
1:D:464:ALA:HA	1:D:467:LEU:HD12	1.85	0.59
1:A:319:PHE:CE2	1:A:407:LEU:HD23	2.38	0.59
1:C:175:ASN:O	1:C:286:SER:HB3	2.03	0.59
1:C:195:VAL:CG2	1:C:198:GLY:C	2.75	0.59
5:H:242:ASN:HB3	5:H:244:ASN:OD1	2.02	0.59
1:A:12:LYS:O	1:A:15:ASN:HB2	2.03	0.58
1:F:464:ALA:HA	1:F:467:LEU:HD12	1.84	0.58
2:B:211:ASN:O	1:D:427:MET:HG3	2.03	0.58
1:A:280:GLN:HE21	1:A:280:GLN:HA	1.68	0.58
4:G:175:ASN:O	4:G:286:SER:HB3	2.03	0.58
1:D:319:PHE:CE2	1:D:407:LEU:HD23	2.38	0.58
1:F:312:ASN:HD22	1:F:312:ASN:N	2.01	0.58
2:B:464:ALA:HA	2:B:467:LEU:HD12	1.85	0.58
1:F:427:MET:HE1	4:G:180:ASP:HB3	1.86	0.58
5:H:17:LEU:HD23	5:H:225:GLN:NE2	2.18	0.58
2:B:175:ASN:O	2:B:286:SER:HB3	2.03	0.58
3:E:451:ILE:HG23	3:E:484:MET:HE1	1.84	0.58
4:G:451:ILE:HG23	4:G:484:MET:HE1	1.85	0.58
5:H:38:LYS:HG3	5:H:38:LYS:O	2.03	0.58
1:A:112:GLN:HE21	7:A:604:GOL:H11	1.68	0.58
1:F:451:ILE:HG23	1:F:484:MET:HE1	1.85	0.58
4:G:509:GLN:HE22	4:G:527:LEU:HA	1.69	0.58
5:H:397:GLN:O	5:H:401:THR:HG23	2.04	0.58
1:A:16:GLY:HA2	1:A:18:PHE:CE1	2.38	0.57
1:A:397:GLN:O	1:A:401:THR:HG23	2.04	0.57
1:A:464:ALA:HA	1:A:467:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:GLN:O	1:C:401:THR:HG23	2.04	0.57
1:D:397:GLN:O	1:D:401:THR:HG23	2.04	0.57
3:E:464:ALA:HA	3:E:467:LEU:HD12	1.85	0.57
2:B:130:ARG:NH1	2:B:158:GLU:OE2	2.34	0.57
4:G:130:ARG:NH2	4:G:158:GLU:HA	2.19	0.57
4:G:464:ALA:HA	4:G:467:LEU:HD12	1.85	0.57
3:E:397:GLN:O	3:E:401:THR:HG23	2.05	0.57
1:A:203:VAL:HG11	1:A:226:GLN:HB3	1.85	0.57
2:B:451:ILE:HG23	2:B:484:MET:HE1	1.86	0.57
1:A:175:ASN:O	1:A:286:SER:HB3	2.03	0.57
1:D:363:ARG:HB3	1:D:392:GLU:CB	2.35	0.57
1:D:365:PRO:HG3	1:D:390:TYR:OH	2.03	0.57
1:C:464:ALA:HA	1:C:467:LEU:HD12	1.86	0.57
1:F:397:GLN:O	1:F:401:THR:HG23	2.04	0.57
4:G:203:VAL:HG11	4:G:226:GLN:HB3	1.85	0.57
5:H:464:ALA:HA	5:H:467:LEU:HD12	1.87	0.57
2:B:397:GLN:O	2:B:401:THR:HG23	2.05	0.56
1:C:199:THR:HG23	5:H:210:LYS:HE3	1.85	0.56
1:D:14:PHE:O	1:D:17:LEU:HB2	2.06	0.56
1:A:138:ARG:NH2	1:A:150:HIS:CE1	2.73	0.56
4:G:397:GLN:O	4:G:401:THR:HG23	2.05	0.56
4:G:38:LYS:O	4:G:38:LYS:HG2	2.05	0.56
1:A:14:PHE:CG	1:A:298:HIS:CE1	2.94	0.56
1:A:112:GLN:NE2	7:A:604:GOL:H11	2.21	0.56
3:E:38:LYS:HG3	3:E:38:LYS:O	2.05	0.56
2:B:494:ARG:HH11	2:B:494:ARG:HG2	1.69	0.56
3:E:512:ALA:O	3:E:514:ARG:N	2.38	0.56
1:F:389:SER:C	1:F:390:TYR:O	2.49	0.55
5:H:451:ILE:HG23	5:H:484:MET:HE1	1.87	0.55
1:C:451:ILE:HG23	1:C:484:MET:HE1	1.89	0.55
4:G:51:ASP:OD2	4:G:53:THR:HG23	2.07	0.55
5:H:512:ALA:O	5:H:514:ARG:N	2.38	0.55
1:F:203:VAL:HG11	1:F:226:GLN:HB3	1.88	0.54
4:G:58:PHE:CD1	4:G:75:PHE:HB2	2.42	0.54
4:G:249:LEU:HD12	4:G:249:LEU:O	2.07	0.54
2:B:512:ALA:O	2:B:514:ARG:N	2.38	0.54
5:H:375:ASP:C	5:H:375:ASP:OD1	2.51	0.54
1:C:145:GLN:O	1:C:146:ALA:CB	2.55	0.54
2:B:58:PHE:CD1	2:B:75:PHE:HB2	2.43	0.54
1:C:275:PRO:HB2	5:H:182:PHE:HB3	1.90	0.54
1:F:363:ARG:HB3	1:F:392:GLU:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:58:PHE:CG	3:E:75:PHE:HB2	2.43	0.54
5:H:58:PHE:CD1	5:H:75:PHE:HB2	2.42	0.54
5:H:58:PHE:CG	5:H:75:PHE:HB2	2.43	0.54
1:A:16:GLY:O	1:A:225:GLN:HG3	2.04	0.54
3:E:478:GLY:HA2	3:E:514:ARG:HH21	1.73	0.54
1:A:451:ILE:HG23	1:A:484:MET:HE1	1.89	0.53
3:E:375:ASP:C	3:E:375:ASP:OD1	2.51	0.53
4:G:512:ALA:C	4:G:514:ARG:H	2.15	0.53
4:G:58:PHE:CG	4:G:75:PHE:HB2	2.43	0.53
1:A:321:ALA:C	1:A:323:ASN:N	2.67	0.53
1:F:321:ALA:O	1:F:322:SER:C	2.52	0.53
3:E:58:PHE:CD1	3:E:75:PHE:HB2	2.42	0.53
1:F:58:PHE:CG	1:F:75:PHE:HB2	2.44	0.53
1:F:513:LEU:O	1:F:514:ARG:C	2.52	0.53
1:D:389:SER:C	1:D:390:TYR:O	2.51	0.53
1:A:58:PHE:CD1	1:A:75:PHE:HB2	2.44	0.53
2:B:58:PHE:CG	2:B:75:PHE:HB2	2.43	0.53
1:D:321:ALA:O	1:D:322:SER:C	2.52	0.52
3:E:182:PHE:N	3:E:182:PHE:CD1	2.74	0.52
1:F:58:PHE:CD1	1:F:75:PHE:HB2	2.43	0.52
1:C:321:ALA:O	1:C:322:SER:C	2.53	0.52
2:B:462:VAL:HG11	2:B:497:SER:HB2	1.91	0.52
1:C:58:PHE:CG	1:C:75:PHE:HB2	2.45	0.52
1:C:130:ARG:NH1	1:C:158:GLU:OE2	2.31	0.52
1:F:390:TYR:HE2	1:F:428:ILE:HD11	1.74	0.52
4:G:512:ALA:O	4:G:514:ARG:N	2.42	0.52
5:H:46:TYR:HA	5:H:55:SER:O	2.10	0.52
1:A:321:ALA:O	1:A:322:SER:C	2.52	0.52
1:D:58:PHE:CG	1:D:75:PHE:HB2	2.45	0.52
3:E:46:TYR:HA	3:E:55:SER:O	2.10	0.52
1:C:199:THR:HG23	5:H:210:LYS:HE2	1.90	0.52
1:F:46:TYR:HA	1:F:55:SER:O	2.10	0.52
1:D:451:ILE:HG23	1:D:484:MET:HE1	1.92	0.52
3:E:512:ALA:C	3:E:514:ARG:H	2.18	0.52
1:C:46:TYR:HA	1:C:55:SER:O	2.10	0.52
1:C:278:ALA:HB1	5:H:177:GLU:CD	2.35	0.52
3:E:130:ARG:NH1	3:E:158:GLU:OE1	2.37	0.52
5:H:321:ALA:C	5:H:323:ASN:N	2.68	0.52
4:G:75:PHE:CZ	4:G:77:VAL:HB	2.45	0.52
1:A:46:TYR:HA	1:A:55:SER:O	2.10	0.52
1:A:510:PHE:CD1	1:A:510:PHE:C	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:ALA:O	2:B:322:SER:C	2.52	0.52
1:C:58:PHE:CD1	1:C:75:PHE:HB2	2.44	0.52
5:H:512:ALA:C	5:H:514:ARG:H	2.18	0.52
2:B:542:ARG:HG3	2:B:543:ASN:H	1.75	0.52
1:D:359:ASP:OD1	1:D:362:LYS:N	2.34	0.52
3:E:182:PHE:N	3:E:182:PHE:HD1	2.08	0.52
4:G:462:VAL:HG11	4:G:497:SER:HB2	1.92	0.52
5:H:321:ALA:O	5:H:322:SER:C	2.52	0.52
1:D:46:TYR:HA	1:D:55:SER:O	2.10	0.51
1:F:510:PHE:CD1	1:F:510:PHE:C	2.87	0.51
1:A:325:ASN:OD1	1:A:327:ARG:NH2	2.40	0.51
1:C:75:PHE:CZ	1:C:77:VAL:HB	2.45	0.51
2:B:321:ALA:C	2:B:323:ASN:N	2.67	0.51
1:D:510:PHE:CD1	1:D:510:PHE:C	2.88	0.51
3:E:321:ALA:O	3:E:322:SER:C	2.52	0.51
4:G:321:ALA:O	4:G:322:SER:C	2.53	0.51
1:C:321:ALA:C	1:C:323:ASN:N	2.67	0.51
1:F:462:VAL:HG11	1:F:497:SER:HB2	1.92	0.51
4:G:321:ALA:C	4:G:323:ASN:N	2.68	0.51
2:B:384:LEU:HB3	2:B:402:SER:HB3	1.93	0.51
1:C:322:SER:HB2	1:C:448:ASP:OD2	2.11	0.51
4:G:46:TYR:HA	4:G:55:SER:O	2.10	0.51
5:H:451:ILE:HD11	5:H:454:LEU:HA	1.93	0.51
2:B:46:TYR:HA	2:B:55:SER:O	2.10	0.51
1:D:512:ALA:O	1:D:514:ARG:N	2.37	0.51
3:E:321:ALA:C	3:E:323:ASN:N	2.68	0.51
5:H:195:VAL:HG12	5:H:199:THR:O	2.11	0.51
1:A:322:SER:HB2	1:A:448:ASP:OD2	2.11	0.51
2:B:113:PHE:HZ	2:B:116:GLU:HB2	1.76	0.51
3:E:147:GLN:HE21	3:E:148:PRO:HD3	1.76	0.51
1:F:321:ALA:C	1:F:323:ASN:N	2.67	0.51
1:A:58:PHE:CG	1:A:75:PHE:HB2	2.44	0.51
3:E:451:ILE:HD11	3:E:454:LEU:HA	1.93	0.51
1:D:321:ALA:C	1:D:323:ASN:N	2.68	0.51
1:D:322:SER:HB2	1:D:448:ASP:OD2	2.11	0.51
1:D:451:ILE:HD11	1:D:454:LEU:HA	1.93	0.51
4:G:509:GLN:NE2	4:G:527:LEU:HA	2.26	0.51
5:H:511:VAL:HG21	5:H:523:VAL:CG1	2.41	0.51
2:B:451:ILE:HD11	2:B:454:LEU:HA	1.92	0.50
1:A:138:ARG:NH2	1:A:150:HIS:HE1	2.09	0.50
5:H:510:PHE:CD1	5:H:510:PHE:C	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:ARG:HH11	2:B:494:ARG:CG	2.24	0.50
3:E:51:ASP:OD2	3:E:53:THR:HG23	2.11	0.50
1:A:321:ALA:C	1:A:323:ASN:H	2.20	0.50
1:C:451:ILE:HD11	1:C:454:LEU:HA	1.93	0.50
1:D:517:GLN:HG3	1:D:520:GLU:CD	2.36	0.50
4:G:319:PHE:HE2	4:G:407:LEU:HD23	1.74	0.50
5:H:322:SER:HB2	5:H:448:ASP:OD2	2.11	0.50
1:D:58:PHE:CD1	1:D:75:PHE:HB2	2.45	0.50
4:G:113:PHE:HZ	4:G:116:GLU:HB2	1.76	0.50
2:B:75:PHE:CZ	2:B:77:VAL:HB	2.47	0.50
3:E:515:ASP:HA	3:E:523:VAL:CG2	2.42	0.50
1:F:322:SER:HB2	1:F:448:ASP:OD2	2.12	0.50
5:H:51:ASP:OD2	5:H:53:THR:HG23	2.11	0.50
1:A:130:ARG:NH2	1:A:158:GLU:OE1	2.36	0.50
2:B:102:ARG:NH2	1:F:99:GLN:O	2.43	0.50
3:E:510:PHE:CD1	3:E:510:PHE:C	2.89	0.50
1:F:512:ALA:O	1:F:514:ARG:N	2.40	0.50
4:G:451:ILE:HD11	4:G:454:LEU:HA	1.93	0.50
1:C:159:GLU:OE1	1:C:164:LYS:HD3	2.12	0.50
3:E:462:VAL:HG11	3:E:497:SER:HB2	1.94	0.50
1:F:75:PHE:CZ	1:F:77:VAL:HB	2.47	0.50
1:A:41:PRO:HG2	1:A:69:PRO:HG3	1.94	0.50
1:A:113:PHE:HZ	1:A:116:GLU:HB2	1.76	0.50
2:B:322:SER:HB2	2:B:448:ASP:OD2	2.11	0.50
2:B:512:ALA:C	2:B:514:ARG:H	2.19	0.50
1:C:325:ASN:OD1	1:C:327:ARG:NH1	2.40	0.50
3:E:31:ARG:HB3	3:E:34:ASP:HB2	1.94	0.50
1:A:64:LEU:HD22	1:A:99:GLN:HG2	1.94	0.49
2:B:321:ALA:O	2:B:323:ASN:N	2.45	0.49
1:A:451:ILE:HD11	1:A:454:LEU:HA	1.92	0.49
1:A:462:VAL:HG11	1:A:497:SER:HB2	1.94	0.49
1:C:113:PHE:HZ	1:C:116:GLU:HB2	1.76	0.49
1:F:451:ILE:HD11	1:F:454:LEU:HA	1.94	0.49
4:G:32:ASP:O	4:G:33:ARG:C	2.54	0.49
5:H:21:ILE:CD1	5:H:125:ILE:HG21	2.42	0.49
3:E:322:SER:HB2	3:E:448:ASP:OD2	2.12	0.49
4:G:384:LEU:HB3	4:G:402:SER:HB3	1.95	0.49
1:C:139:LYS:HB3	4:G:455:GLN:HG2	1.93	0.49
1:A:318:ASP:C	1:A:318:ASP:OD1	2.55	0.49
1:A:321:ALA:O	1:A:323:ASN:N	2.45	0.49
4:G:322:SER:HB2	4:G:448:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:462:VAL:HG11	5:H:497:SER:HB2	1.94	0.49
1:A:16:GLY:HA2	1:A:18:PHE:HE1	1.78	0.49
1:D:113:PHE:HZ	1:D:116:GLU:HB2	1.77	0.49
1:D:462:VAL:HG11	1:D:497:SER:HB2	1.93	0.49
3:E:75:PHE:CZ	3:E:77:VAL:HB	2.47	0.49
4:G:312:ASN:HB3	4:G:441:TYR:CD1	2.48	0.49
1:A:75:PHE:CZ	1:A:77:VAL:HB	2.47	0.49
2:B:165:ILE:O	2:B:224:VAL:HG22	2.13	0.49
1:C:227:VAL:HG12	1:C:234:VAL:HG11	1.95	0.49
1:C:318:ASP:OD1	1:C:318:ASP:C	2.56	0.49
1:F:17:LEU:HB3	1:F:225:GLN:OE1	2.12	0.49
1:F:113:PHE:HZ	1:F:116:GLU:HB2	1.77	0.49
1:F:318:ASP:C	1:F:318:ASP:OD1	2.55	0.49
5:H:75:PHE:CZ	5:H:77:VAL:HB	2.47	0.49
2:B:182:PHE:CD2	2:B:182:PHE:C	2.90	0.49
2:B:312:ASN:HB3	2:B:441:TYR:CD1	2.48	0.49
1:D:130:ARG:NH1	1:D:158:GLU:OE2	2.31	0.49
1:D:363:ARG:HB2	1:D:392:GLU:OE1	2.13	0.49
1:F:312:ASN:N	1:F:312:ASN:ND2	2.60	0.49
5:H:319:PHE:HE2	5:H:407:LEU:HD23	1.76	0.49
1:A:277:GLY:C	1:A:279:GLY:N	2.71	0.48
1:C:312:ASN:HB3	1:C:441:TYR:CD1	2.48	0.48
1:C:462:VAL:HG11	1:C:497:SER:HB2	1.93	0.48
1:C:516:VAL:O	1:C:517:GLN:HB2	2.12	0.48
1:D:75:PHE:CZ	1:D:77:VAL:HB	2.48	0.48
1:F:21:ILE:CD1	1:F:125:ILE:HG21	2.42	0.48
1:D:318:ASP:C	1:D:318:ASP:OD1	2.56	0.48
5:H:196:GLU:C	5:H:198:GLY:H	2.21	0.48
1:C:64:LEU:HD22	1:C:99:GLN:HG2	1.95	0.48
1:F:321:ALA:O	1:F:323:ASN:N	2.45	0.48
5:H:113:PHE:HZ	5:H:116:GLU:HB2	1.78	0.48
1:A:512:ALA:O	1:A:514:ARG:N	2.43	0.48
4:G:321:ALA:O	4:G:323:ASN:N	2.47	0.48
3:E:321:ALA:O	3:E:323:ASN:N	2.47	0.48
1:F:319:PHE:HE2	1:F:407:LEU:HD23	1.79	0.48
5:H:326:PRO:HD3	5:H:412:LEU:HD11	1.96	0.48
1:A:21:ILE:CD1	1:A:125:ILE:HG21	2.41	0.48
2:B:318:ASP:OD1	2:B:318:ASP:C	2.56	0.48
1:C:321:ALA:O	1:C:323:ASN:N	2.45	0.48
3:E:319:PHE:HE2	3:E:407:LEU:HD23	1.76	0.48
5:H:312:ASN:HB3	5:H:441:TYR:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:318:ASP:OD1	5:H:318:ASP:C	2.56	0.48
5:H:321:ALA:O	5:H:323:ASN:N	2.46	0.48
2:B:321:ALA:C	2:B:323:ASN:H	2.21	0.48
3:E:312:ASN:HB3	3:E:441:TYR:CD1	2.49	0.48
1:A:312:ASN:HB3	1:A:441:TYR:CD1	2.49	0.48
2:B:303:GLU:OE1	1:F:261:GLU:CD	2.57	0.48
1:D:321:ALA:O	1:D:323:ASN:N	2.46	0.48
3:E:318:ASP:OD1	3:E:318:ASP:C	2.57	0.48
4:G:102:ARG:HH22	4:G:105:MET:HE3	1.79	0.48
3:E:113:PHE:HZ	3:E:116:GLU:HB2	1.78	0.48
5:H:542:ARG:O	5:H:543:ASN:CB	2.60	0.47
1:D:140:ASP:C	1:D:142:PHE:N	2.72	0.47
3:E:21:ILE:CD1	3:E:125:ILE:HG21	2.40	0.47
1:F:17:LEU:HB3	1:F:225:GLN:CD	2.38	0.47
1:F:321:ALA:C	1:F:323:ASN:H	2.21	0.47
1:F:514:ARG:HG3	1:F:515:ASP:N	2.28	0.47
4:G:321:ALA:C	4:G:323:ASN:H	2.22	0.47
1:C:321:ALA:C	1:C:323:ASN:H	2.21	0.47
5:H:511:VAL:HG21	5:H:523:VAL:HG12	1.95	0.47
1:D:64:LEU:HD22	1:D:99:GLN:HG2	1.97	0.47
3:E:31:ARG:HB3	3:E:34:ASP:CB	2.44	0.47
3:E:384:LEU:HB3	3:E:402:SER:HB3	1.95	0.47
1:F:64:LEU:HD22	1:F:99:GLN:HG2	1.97	0.47
4:G:318:ASP:OD1	4:G:318:ASP:C	2.57	0.47
5:H:227:VAL:HG12	5:H:234:VAL:HG11	1.96	0.47
5:H:542:ARG:HG2	5:H:543:ASN:N	2.29	0.47
2:B:303:GLU:OE1	1:F:261:GLU:OE2	2.32	0.47
1:C:223:SER:OG	1:C:226:GLN:HG3	2.14	0.47
1:F:390:TYR:CE2	1:F:428:ILE:HD11	2.49	0.47
5:H:139:LYS:O	5:H:139:LYS:HG3	2.13	0.47
5:H:321:ALA:C	5:H:323:ASN:H	2.22	0.47
1:C:521:ILE:HG22	1:C:522:SER:N	2.28	0.47
1:A:14:PHE:HD1	1:A:14:PHE:H	1.62	0.47
1:C:319:PHE:HE2	1:C:407:LEU:HD23	1.80	0.47
1:D:262:LYS:NZ	4:G:128:SER:O	2.48	0.47
1:F:325:ASN:OD1	1:F:327:ARG:NH1	2.39	0.47
2:B:41:PRO:HG2	2:B:69:PRO:HG3	1.97	0.47
1:C:21:ILE:CD1	1:C:125:ILE:HG21	2.42	0.47
1:C:201:ILE:O	1:C:203:VAL:HG23	2.15	0.47
1:D:21:ILE:CD1	1:D:125:ILE:HG21	2.44	0.47
1:F:8:TYR:CZ	1:F:13:GLY:HA2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:385:ASN:ND2	1:F:391:SER:HB3	2.18	0.47
1:D:321:ALA:C	1:D:323:ASN:H	2.22	0.47
3:E:321:ALA:C	3:E:323:ASN:H	2.23	0.47
3:E:376:ALA:HB1	3:E:377:PRO:HD2	1.97	0.47
1:F:41:PRO:HG2	1:F:69:PRO:HG3	1.95	0.47
2:B:21:ILE:CD1	2:B:125:ILE:HG21	2.43	0.47
2:B:223:SER:O	2:B:227:VAL:HG12	2.16	0.47
3:E:181:LEU:N	3:E:181:LEU:HD12	2.30	0.47
5:H:376:ALA:HB1	5:H:377:PRO:HD2	1.97	0.47
1:D:-8:THR:O	1:D:-7:SER:HB3	2.15	0.46
3:E:521:ILE:HB	3:E:525:GLN:NE2	2.30	0.46
4:G:130:ARG:HD3	4:G:306:ALA:HB2	1.97	0.46
4:G:184:LYS:NZ	4:G:242:ASN:ND2	2.62	0.46
5:H:516:VAL:O	5:H:517:GLN:HB2	2.16	0.46
1:C:-8:THR:O	1:C:-7:SER:HB3	2.15	0.46
1:D:17:LEU:CA	1:D:225:GLN:HE22	2.28	0.46
1:D:363:ARG:HB3	1:D:392:GLU:CD	2.40	0.46
1:A:201:ILE:O	1:A:203:VAL:HG23	2.16	0.46
2:B:223:SER:OG	2:B:226:GLN:HG3	2.15	0.46
3:E:181:LEU:C	3:E:183:SER:H	2.23	0.46
1:D:383:ASN:HB3	1:D:385:ASN:HD22	1.76	0.46
4:G:277:GLY:HA2	4:G:280:GLN:O	2.16	0.46
5:H:-8:THR:O	5:H:-7:SER:HB3	2.16	0.46
5:H:223:SER:OG	5:H:226:GLN:HG3	2.16	0.46
2:B:102:ARG:HH22	2:B:105:MET:HE3	1.80	0.46
1:D:181:LEU:HD22	5:H:385:ASN:O	2.15	0.46
1:F:201:ILE:O	1:F:203:VAL:HG23	2.16	0.46
4:G:102:ARG:HH22	4:G:105:MET:CE	2.29	0.46
2:B:201:ILE:O	2:B:203:VAL:HG23	2.15	0.46
1:D:223:SER:OG	1:D:226:GLN:HG3	2.15	0.46
3:E:201:ILE:O	3:E:203:VAL:HG23	2.16	0.46
3:E:227:VAL:HG12	3:E:234:VAL:HG11	1.98	0.46
4:G:21:ILE:CD1	4:G:125:ILE:HG21	2.43	0.46
4:G:223:SER:OG	4:G:226:GLN:HG3	2.16	0.46
5:H:196:GLU:OE1	5:H:196:GLU:HA	2.15	0.46
1:A:18:PHE:HB2	1:A:225:GLN:HE21	1.80	0.46
1:A:223:SER:OG	1:A:226:GLN:HG3	2.15	0.46
4:G:31:ARG:HB3	4:G:67:LEU:HD21	1.95	0.46
5:H:201:ILE:O	5:H:203:VAL:HG23	2.15	0.46
1:C:195:VAL:HG21	1:C:198:GLY:C	2.40	0.45
1:F:513:LEU:O	1:F:514:ARG:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:199:THR:HA	5:H:200:PRO:HD3	1.86	0.45
5:H:384:LEU:HB3	5:H:402:SER:HB3	1.97	0.45
1:D:461:LEU:HD22	1:D:508:VAL:CG2	2.46	0.45
3:E:223:SER:OG	3:E:226:GLN:HG3	2.17	0.45
1:D:336:ASP:OD2	1:D:338:SER:OG	2.21	0.45
4:G:201:ILE:O	4:G:203:VAL:HG23	2.15	0.45
1:D:44:VAL:HG12	1:D:46:TYR:CE1	2.52	0.45
1:D:376:ALA:HB1	1:D:377:PRO:HD2	1.99	0.45
5:H:31:ARG:C	5:H:33:ARG:H	2.24	0.45
1:A:14:PHE:CD1	1:A:14:PHE:N	2.85	0.45
1:A:102:ARG:HH22	1:A:105:MET:CE	2.30	0.45
1:C:41:PRO:HG2	1:C:69:PRO:HG3	1.97	0.45
1:D:201:ILE:O	1:D:203:VAL:HG23	2.16	0.45
3:E:326:PRO:HD3	3:E:412:LEU:HD11	1.99	0.45
4:G:376:ALA:HB1	4:G:377:PRO:HD2	1.99	0.45
5:H:301:PHE:CE2	5:H:305:LEU:HD11	2.52	0.45
1:F:-8:THR:O	1:F:-7:SER:HB3	2.17	0.45
1:F:363:ARG:HB3	1:F:392:GLU:CB	2.46	0.45
1:A:461:LEU:HD22	1:A:508:VAL:CG2	2.47	0.45
2:B:326:PRO:HD3	2:B:412:LEU:HD11	1.98	0.45
2:B:461:LEU:HD22	2:B:508:VAL:CG2	2.47	0.45
1:D:41:PRO:HG2	1:D:69:PRO:HG3	1.97	0.45
1:F:514:ARG:CG	1:F:515:ASP:N	2.77	0.45
4:G:266:ALA:HB1	4:G:268:GLN:HE21	1.82	0.45
1:D:144:PRO:HB2	1:D:145:GLN:H	1.65	0.45
2:B:522:SER:OG	2:B:524:VAL:HG22	2.17	0.45
3:E:41:PRO:HG2	3:E:69:PRO:HG3	1.98	0.45
1:A:384:LEU:HB3	1:A:402:SER:HB3	1.99	0.44
1:D:325:ASN:OD1	1:D:327:ARG:NH2	2.50	0.44
3:E:417:LEU:HD22	3:E:453:ASP:HB3	1.99	0.44
1:F:384:LEU:HB3	1:F:402:SER:HB3	1.99	0.44
1:D:11:SER:O	1:D:12:LYS:HD2	2.18	0.44
3:E:301:PHE:CE2	3:E:305:LEU:HD11	2.52	0.44
1:F:102:ARG:HH22	1:F:105:MET:CE	2.30	0.44
2:B:297:VAL:HB	1:F:295:GLU:CB	2.42	0.44
2:B:319:PHE:HE2	2:B:384:LEU:HD21	1.81	0.44
1:D:285:LYS:CE	5:H:389:SER:HB2	2.39	0.44
2:B:58:PHE:CG	2:B:59:ARG:N	2.86	0.44
1:C:384:LEU:HB3	1:C:402:SER:HB3	2.00	0.44
1:D:199:THR:HA	1:D:200:PRO:HD3	1.83	0.44
1:F:44:VAL:HG12	1:F:46:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-8:THR:O	1:A:-7:SER:HB3	2.16	0.44
1:C:319:PHE:HB3	1:C:371:ALA:HB2	1.98	0.44
3:E:31:ARG:HG3	3:E:114:LEU:HD22	1.99	0.44
3:E:32:ASP:HB2	3:E:149:HIS:HD2	1.81	0.44
1:D:312:ASN:HB2	1:D:441:TYR:CD1	2.53	0.44
4:G:249:LEU:CD1	4:G:274:LEU:HD21	2.44	0.44
1:F:376:ALA:HB1	1:F:377:PRO:HD2	2.00	0.44
4:G:326:PRO:HD3	4:G:412:LEU:HD11	1.99	0.44
1:A:319:PHE:HB3	1:A:371:ALA:HB2	1.99	0.44
2:B:223:SER:OG	2:B:225:GLN:HG2	2.18	0.44
1:F:542:ARG:HG2	1:F:543:ASN:N	2.32	0.44
1:D:101:SER:HA	4:G:100:ASN:O	2.18	0.43
1:D:510:PHE:CD1	1:D:511:VAL:N	2.86	0.43
2:B:253:VAL:HG22	2:B:254:GLN:N	2.32	0.43
1:F:326:PRO:HD3	1:F:412:LEU:HD11	2.00	0.43
1:A:510:PHE:CD1	1:A:511:VAL:N	2.86	0.43
1:C:14:PHE:HD1	1:C:14:PHE:H	1.65	0.43
4:G:319:PHE:HB3	4:G:371:ALA:HB2	2.00	0.43
5:H:223:SER:O	5:H:227:VAL:HG22	2.19	0.43
2:B:102:ARG:HH22	2:B:105:MET:CE	2.32	0.43
1:C:58:PHE:CG	1:C:59:ARG:N	2.86	0.43
1:F:199:THR:HA	1:F:200:PRO:HD3	1.86	0.43
1:F:314:MET:HG2	1:F:365:PRO:HG2	2.00	0.43
1:A:58:PHE:CG	1:A:59:ARG:N	2.87	0.43
1:D:326:PRO:HD3	1:D:412:LEU:HD11	2.00	0.43
1:F:142:PHE:C	1:F:144:PRO:HD3	2.36	0.43
1:F:510:PHE:CD1	1:F:511:VAL:N	2.86	0.43
4:G:249:LEU:HD12	4:G:274:LEU:HD21	1.99	0.43
5:H:461:LEU:HD22	5:H:508:VAL:CG2	2.49	0.43
1:C:461:LEU:HD22	1:C:508:VAL:CG2	2.48	0.43
1:F:535:PHE:CZ	1:F:539:MET:HE3	2.54	0.43
1:A:301:PHE:CE2	1:A:305:LEU:HD11	2.54	0.43
4:G:58:PHE:CG	4:G:59:ARG:N	2.87	0.43
1:C:376:ALA:HB1	1:C:377:PRO:HD2	2.01	0.43
3:E:461:LEU:HD22	3:E:508:VAL:CG2	2.49	0.43
4:G:461:LEU:HD22	4:G:508:VAL:CG2	2.48	0.43
5:H:41:PRO:HG2	5:H:69:PRO:HG3	2.01	0.43
1:A:18:PHE:HB2	1:A:225:GLN:NE2	2.34	0.43
2:B:376:ALA:HB1	2:B:377:PRO:HD2	2.01	0.43
1:C:140:ASP:CG	1:C:148:PRO:HD2	2.44	0.43
5:H:510:PHE:CD1	5:H:511:VAL:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:ARG:HH22	1:F:105:MET:HE2	1.84	0.43
4:G:511:VAL:HG21	4:G:523:VAL:CG1	2.49	0.43
4:G:435:GLN:O	4:G:435:GLN:CD	2.61	0.42
1:A:102:ARG:HH22	1:A:105:MET:HE3	1.85	0.42
2:B:494:ARG:CG	2:B:494:ARG:NH1	2.82	0.42
1:C:314:MET:HG2	1:C:365:PRO:HG2	2.01	0.42
5:H:58:PHE:CG	5:H:59:ARG:N	2.87	0.42
2:B:301:PHE:CE2	2:B:305:LEU:HD11	2.54	0.42
2:B:314:MET:HB2	2:B:443:LEU:HA	2.02	0.42
1:D:152:LYS:HB2	1:D:152:LYS:HE3	1.76	0.42
3:E:199:THR:HA	3:E:200:PRO:HD3	1.85	0.42
2:B:524:VAL:CG2	2:B:525:GLN:N	2.82	0.42
1:C:-7:SER:HB2	1:C:243:SER:HB3	2.02	0.42
3:E:510:PHE:CD1	3:E:511:VAL:N	2.87	0.42
4:G:275:PRO:HA	4:G:281:ASN:CG	2.45	0.42
1:A:12:LYS:HD3	1:A:12:LYS:HA	1.70	0.42
1:A:407:LEU:HD23	1:A:407:LEU:HA	1.87	0.42
2:B:524:VAL:HG23	2:B:525:GLN:N	2.35	0.42
1:C:326:PRO:HD3	1:C:412:LEU:HD11	2.01	0.42
1:D:58:PHE:CG	1:D:59:ARG:N	2.87	0.42
3:E:58:PHE:CG	3:E:59:ARG:N	2.87	0.42
5:H:-7:SER:HB2	5:H:243:SER:HB3	2.01	0.42
5:H:319:PHE:HB3	5:H:371:ALA:HB2	2.01	0.42
1:A:376:ALA:HB1	1:A:377:PRO:HD2	2.01	0.42
3:E:511:VAL:HG21	3:E:523:VAL:CG1	2.50	0.42
4:G:301:PHE:CE2	4:G:305:LEU:HD11	2.54	0.42
1:C:407:LEU:HD23	1:C:407:LEU:HA	1.87	0.42
1:D:440:TYR:HA	1:D:468:PRO:HB2	2.02	0.42
1:F:58:PHE:CG	1:F:59:ARG:N	2.87	0.42
1:F:319:PHE:HB3	1:F:371:ALA:HB2	2.01	0.42
4:G:199:THR:HA	4:G:200:PRO:HD3	1.85	0.42
1:A:319:PHE:HE2	1:A:407:LEU:HD23	1.82	0.42
1:C:143:ALA:HB3	1:C:144:PRO:HD3	2.01	0.42
1:C:301:PHE:CE2	1:C:305:LEU:HD11	2.55	0.42
1:D:31:ARG:NH2	1:D:149:HIS:HB2	2.35	0.42
1:A:44:VAL:HG12	1:A:46:TYR:CE1	2.54	0.41
1:A:138:ARG:CZ	1:A:150:HIS:CE1	3.03	0.41
1:D:301:PHE:CE2	1:D:305:LEU:HD11	2.55	0.41
1:F:312:ASN:HB2	1:F:441:TYR:CD1	2.55	0.41
1:A:200:PRO:O	1:A:202:PRO:HD3	2.21	0.41
1:C:-2:ILE:O	1:C:1:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:LEU:HB3	1:F:114:LEU:HD13	2.01	0.41
4:G:130:ARG:HH22	4:G:158:GLU:HA	1.83	0.41
1:D:465:SER:HA	1:D:507:ILE:HD13	2.02	0.41
1:A:277:GLY:O	1:A:280:GLN:N	2.38	0.41
1:A:326:PRO:HD3	1:A:412:LEU:HD11	2.01	0.41
3:E:223:SER:O	3:E:227:VAL:HG22	2.21	0.41
4:G:37:SER:O	4:G:38:LYS:C	2.64	0.41
4:G:417:LEU:HD22	4:G:453:ASP:HB3	2.03	0.41
1:D:-2:ILE:O	1:D:1:THR:HG22	2.21	0.41
1:D:319:PHE:HB3	1:D:371:ALA:HB2	2.02	0.41
5:H:465:SER:HA	5:H:507:ILE:HD13	2.03	0.41
2:B:441:TYR:O	2:B:469:LEU:HA	2.21	0.41
1:D:314:MET:HG2	1:D:365:PRO:HG2	2.01	0.41
3:E:441:TYR:O	3:E:469:LEU:HA	2.21	0.41
5:H:149:HIS:ND1	5:H:149:HIS:N	2.69	0.41
5:H:314:MET:HB2	5:H:443:LEU:HA	2.03	0.41
1:C:44:VAL:HG12	1:C:46:TYR:CE1	2.56	0.41
1:F:7:TYR:CZ	1:F:494:ARG:HG3	2.56	0.41
1:F:144:PRO:HB2	1:F:145:GLN:H	1.63	0.41
4:G:41:PRO:HG2	4:G:69:PRO:HG3	2.01	0.41
5:H:441:TYR:O	5:H:469:LEU:HA	2.21	0.41
2:B:188:PHE:CD2	2:B:208:VAL:HG22	2.56	0.41
2:B:478:GLY:CA	2:B:514:ARG:HH21	2.29	0.41
1:C:30:LEU:HB3	1:C:114:LEU:HD13	2.02	0.41
1:C:384:LEU:HD23	1:C:384:LEU:HA	1.92	0.41
1:C:417:LEU:HD22	1:C:453:ASP:HB3	2.01	0.41
1:C:465:SER:HA	1:C:507:ILE:HD13	2.03	0.41
3:E:319:PHE:HB3	3:E:371:ALA:HB2	2.03	0.41
4:G:184:LYS:HZ1	4:G:242:ASN:ND2	2.19	0.41
4:G:515:ASP:OD1	4:G:515:ASP:N	2.53	0.41
2:B:465:SER:HA	2:B:507:ILE:HD13	2.02	0.41
1:C:14:PHE:CD1	1:C:14:PHE:N	2.89	0.41
1:D:-7:SER:HB2	1:D:243:SER:HB3	2.03	0.41
1:F:407:LEU:HD23	1:F:407:LEU:HA	1.87	0.41
4:G:511:VAL:HG21	4:G:523:VAL:HG12	2.03	0.41
3:E:31:ARG:HE	3:E:31:ARG:HB2	1.69	0.40
1:F:-7:SER:HB2	1:F:243:SER:HB3	2.03	0.40
1:F:301:PHE:CE2	1:F:305:LEU:HD11	2.55	0.40
4:G:307:SER:O	4:G:438:ARG:NH1	2.55	0.40
5:H:44:VAL:HG12	5:H:46:TYR:CE1	2.56	0.40
1:A:14:PHE:HD1	1:A:14:PHE:N	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:SER:O	1:C:227:VAL:HG22	2.21	0.40
1:C:438:ARG:HH11	1:C:438:ARG:HD3	1.76	0.40
1:C:441:TYR:O	1:C:469:LEU:HA	2.21	0.40
1:F:-2:ILE:O	1:F:1:THR:HG22	2.21	0.40
1:F:441:TYR:O	1:F:469:LEU:HA	2.21	0.40
4:G:441:TYR:O	4:G:469:LEU:HA	2.22	0.40
1:A:441:TYR:O	1:A:469:LEU:HA	2.21	0.40
1:C:314:MET:HB2	1:C:443:LEU:HA	2.03	0.40
1:A:-2:ILE:O	1:A:1:THR:HG22	2.20	0.40
1:D:441:TYR:O	1:D:469:LEU:HA	2.21	0.40
1:F:417:LEU:HD22	1:F:453:ASP:HB3	2.02	0.40
1:F:461:LEU:HD22	1:F:508:VAL:CG2	2.51	0.40
4:G:432:SER:OG	4:G:437:SER:HB3	2.22	0.40
4:G:535:PHE:CZ	4:G:539:MET:HE3	2.56	0.40
1:A:374:ILE:O	1:A:375:ASP:HB2	2.21	0.40
1:C:12:LYS:HA	1:C:15:ASN:HD21	1.87	0.40
1:D:513:LEU:O	1:D:514:ARG:O	2.38	0.40
1:F:318:ASP:HB3	1:F:447:THR:HB	2.01	0.40
1:F:432:SER:OG	1:F:437:SER:HB3	2.22	0.40
4:G:451:ILE:HG23	4:G:484:MET:CE	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	542/553 (98%)	504 (93%)	35 (6%)	3 (1%)	21	39
1	C	551/553 (100%)	503 (91%)	40 (7%)	8 (2%)	8	17
1	D	551/553 (100%)	510 (93%)	30 (5%)	11 (2%)	6	12
1	F	551/553 (100%)	510 (93%)	32 (6%)	9 (2%)	7	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	494/528 (94%)	463 (94%)	26 (5%)	5 (1%)	12	24
3	E	526/548 (96%)	487 (93%)	31 (6%)	8 (2%)	8	17
4	G	494/526 (94%)	465 (94%)	27 (6%)	2 (0%)	30	48
5	H	535/553 (97%)	494 (92%)	38 (7%)	3 (1%)	21	39
All	All	4244/4367 (97%)	3936 (93%)	259 (6%)	49 (1%)	10	22

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ALA
2	B	280	GLN
1	C	18	PHE
1	C	146	ALA
1	D	144	PRO
1	D	390	TYR
1	D	514	ARG
1	D	542	ARG
3	E	149	HIS
3	E	276	THR
1	F	12	LYS
1	F	144	PRO
1	F	390	TYR
1	F	514	ARG
1	F	517	GLN
1	A	322	SER
2	B	322	SER
1	C	145	GLN
1	C	322	SER
1	C	517	GLN
1	D	141	GLY
1	D	278	ALA
1	D	322	SER
3	E	150	HIS
3	E	322	SER
3	E	513	LEU
1	F	143	ALA
1	F	322	SER
4	G	322	SER
5	H	322	SER
2	B	17	LEU
2	B	513	LEU

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Mol	Chain	Res	Type
1	C	141	GLY
4	G	513	LEU
5	H	513	LEU
5	H	517	GLN
1	A	513	LEU
1	C	15	ASN
1	C	147	GLN
1	D	381	CYS
1	D	517	GLN
3	E	35	VAL
1	D	513	LEU
1	F	381	CYS
2	B	381	CYS
3	E	36	LEU
3	E	182	PHE
1	F	513	LEU
1	D	277	GLY

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	475/481 (99%)	427 (90%)	48 (10%)	7	15
1	C	481/481 (100%)	433 (90%)	48 (10%)	7	16
1	D	481/481 (100%)	434 (90%)	47 (10%)	7	17
1	F	481/481 (100%)	437 (91%)	44 (9%)	9	20
2	B	441/461 (96%)	393 (89%)	48 (11%)	6	12
3	E	467/477 (98%)	424 (91%)	43 (9%)	8	19
4	G	442/460 (96%)	400 (90%)	42 (10%)	8	18
5	H	474/481 (98%)	427 (90%)	47 (10%)	7	16
All	All	3742/3803 (98%)	3375 (90%)	367 (10%)	7	17

All (367) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	12	LYS
1	A	14	PHE
1	A	17	LEU
1	A	19	SER
1	A	37	SER
1	A	39	SER
1	A	50	LYS
1	A	53	THR
1	A	70	LYS
1	A	77	VAL
1	A	83	THR
1	A	109	ASP
1	A	122	SER
1	A	139	LYS
1	A	147	GLN
1	A	158	GLU
1	A	174	SER
1	A	195	VAL
1	A	202	PRO
1	A	220	VAL
1	A	224	VAL
1	A	225	GLN
1	A	227	VAL
1	A	246	LYS
1	A	252	LYS
1	A	257	LEU
1	A	258	SER
1	A	276	THR
1	A	280	GLN
1	A	285	LYS
1	A	296	THR
1	A	307	SER
1	A	318	ASP
1	A	340	ARG
1	A	389	SER
1	A	397	GLN
1	A	401	THR
1	A	456	GLU
1	A	486	ILE
1	A	491	LYS
1	A	494	ARG
1	A	504	SER

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Mol	Chain	Res	Type
1	A	523	VAL
1	A	524	VAL
1	A	525	GLN
1	A	533	SER
1	A	541	ILE
2	B	17	LEU
2	B	39	SER
2	B	48	LYS
2	B	53	THR
2	B	54	LEU
2	B	70	LYS
2	B	77	VAL
2	B	83	THR
2	B	122	SER
2	B	166	SER
2	B	174	SER
2	B	179	LYS
2	B	181	LEU
2	B	184	LYS
2	B	185	SER
2	B	205	LYS
2	B	210	LYS
2	B	220	VAL
2	B	224	VAL
2	B	225	GLN
2	B	227	VAL
2	B	243	SER
2	B	252	LYS
2	B	257	LEU
2	B	258	SER
2	B	268	GLN
2	B	276	THR
2	B	280	GLN
2	B	282	LYS
2	B	285	LYS
2	B	294	THR
2	B	295	GLU
2	B	296	THR
2	B	298	HIS
2	B	307	SER
2	B	389	SER
2	B	397	GLN

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Mol	Chain	Res	Type
2	B	401	THR
2	B	456	GLU
2	B	486	ILE
2	B	494	ARG
2	B	501	ARG
2	B	504	SER
2	B	530	GLU
2	B	533	SER
2	B	541	ILE
2	B	542	ARG
2	B	543	ASN
1	C	12	LYS
1	C	14	PHE
1	C	17	LEU
1	C	18	PHE
1	C	36	LEU
1	C	37	SER
1	C	39	SER
1	C	53	THR
1	C	70	LYS
1	C	77	VAL
1	C	83	THR
1	C	109	ASP
1	C	122	SER
1	C	130	ARG
1	C	160	SER
1	C	163	SER
1	C	174	SER
1	C	196	GLU
1	C	197	HIS
1	C	220	VAL
1	C	224	VAL
1	C	227	VAL
1	C	252	LYS
1	C	257	LEU
1	C	258	SER
1	C	268	GLN
1	C	276	THR
1	C	294	THR
1	C	296	THR
1	C	307	SER
1	C	318	ASP

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Mol	Chain	Res	Type
1	C	340	ARG
1	C	389	SER
1	C	397	GLN
1	C	401	THR
1	C	427	MET
1	C	456	GLU
1	C	482	LYS
1	C	486	ILE
1	C	491	LYS
1	C	494	ARG
1	C	504	SER
1	C	514	ARG
1	C	515	ASP
1	C	524	VAL
1	C	533	SER
1	C	541	ILE
1	C	542	ARG
1	D	12	LYS
1	D	14	PHE
1	D	15	ASN
1	D	36	LEU
1	D	37	SER
1	D	39	SER
1	D	53	THR
1	D	70	LYS
1	D	77	VAL
1	D	83	THR
1	D	109	ASP
1	D	122	SER
1	D	130	ARG
1	D	152	LYS
1	D	174	SER
1	D	195	VAL
1	D	196	GLU
1	D	199	THR
1	D	220	VAL
1	D	224	VAL
1	D	246	LYS
1	D	252	LYS
1	D	257	LEU
1	D	258	SER
1	D	280	GLN

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Mol	Chain	Res	Type
1	D	294	THR
1	D	296	THR
1	D	307	SER
1	D	318	ASP
1	D	346	ARG
1	D	359	ASP
1	D	385	ASN
1	D	389	SER
1	D	391	SER
1	D	397	GLN
1	D	401	THR
1	D	456	GLU
1	D	486	ILE
1	D	493	GLU
1	D	494	ARG
1	D	504	SER
1	D	515	ASP
1	D	517	GLN
1	D	521	ILE
1	D	524	VAL
1	D	533	SER
1	D	541	ILE
3	E	12	LYS
3	E	17	LEU
3	E	36	LEU
3	E	39	SER
3	E	50	LYS
3	E	54	LEU
3	E	70	LYS
3	E	77	VAL
3	E	83	THR
3	E	109	ASP
3	E	122	SER
3	E	147	GLN
3	E	174	SER
3	E	179	LYS
3	E	183	SER
3	E	195	VAL
3	E	220	VAL
3	E	224	VAL
3	E	225	GLN
3	E	227	VAL

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Mol	Chain	Res	Type
3	E	257	LEU
3	E	258	SER
3	E	285	LYS
3	E	296	THR
3	E	298	HIS
3	E	307	SER
3	E	318	ASP
3	E	327	ARG
3	E	340	ARG
3	E	375	ASP
3	E	389	SER
3	E	397	GLN
3	E	401	THR
3	E	458	LYS
3	E	486	ILE
3	E	491	LYS
3	E	504	SER
3	E	515	ASP
3	E	516	VAL
3	E	524	VAL
3	E	525	GLN
3	E	533	SER
3	E	541	ILE
1	F	-5	MET
1	F	12	LYS
1	F	17	LEU
1	F	36	LEU
1	F	37	SER
1	F	39	SER
1	F	50	LYS
1	F	53	THR
1	F	77	VAL
1	F	83	THR
1	F	104	GLU
1	F	109	ASP
1	F	122	SER
1	F	142	PHE
1	F	174	SER
1	F	195	VAL
1	F	196	GLU
1	F	220	VAL
1	F	224	VAL

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Mol	Chain	Res	Type
1	F	225	GLN
1	F	252	LYS
1	F	257	LEU
1	F	258	SER
1	F	280	GLN
1	F	285	LYS
1	F	296	THR
1	F	307	SER
1	F	312	ASN
1	F	318	ASP
1	F	340	ARG
1	F	363	ARG
1	F	389	SER
1	F	391	SER
1	F	397	GLN
1	F	401	THR
1	F	427	MET
1	F	482	LYS
1	F	486	ILE
1	F	491	LYS
1	F	504	SER
1	F	517	GLN
1	F	524	VAL
1	F	533	SER
1	F	541	ILE
4	G	37	SER
4	G	38	LYS
4	G	39	SER
4	G	70	LYS
4	G	77	VAL
4	G	83	THR
4	G	101	SER
4	G	109	ASP
4	G	122	SER
4	G	138	ARG
4	G	149	HIS
4	G	166	SER
4	G	174	SER
4	G	184	LYS
4	G	185	SER
4	G	195	VAL
4	G	220	VAL

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Mol	Chain	Res	Type
4	G	224	VAL
4	G	225	GLN
4	G	246	LYS
4	G	248	SER
4	G	252	LYS
4	G	257	LEU
4	G	258	SER
4	G	276	THR
4	G	285	LYS
4	G	296	THR
4	G	307	SER
4	G	318	ASP
4	G	327	ARG
4	G	389	SER
4	G	397	GLN
4	G	401	THR
4	G	407	LEU
4	G	486	ILE
4	G	504	SER
4	G	514	ARG
4	G	515	ASP
4	G	524	VAL
4	G	533	SER
4	G	541	ILE
4	G	542	ARG
5	H	10	LYS
5	H	12	LYS
5	H	17	LEU
5	H	32	ASP
5	H	37	SER
5	H	38	LYS
5	H	39	SER
5	H	54	LEU
5	H	67	LEU
5	H	70	LYS
5	H	77	VAL
5	H	83	THR
5	H	109	ASP
5	H	122	SER
5	H	138	ARG
5	H	139	LYS
5	H	149	HIS

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Mol	Chain	Res	Type
5	H	174	SER
5	H	182	PHE
5	H	220	VAL
5	H	224	VAL
5	H	227	VAL
5	H	257	LEU
5	H	258	SER
5	H	276	THR
5	H	285	LYS
5	H	292	LYS
5	H	294	THR
5	H	296	THR
5	H	307	SER
5	H	318	ASP
5	H	327	ARG
5	H	375	ASP
5	H	389	SER
5	H	397	GLN
5	H	401	THR
5	H	407	LEU
5	H	456	GLU
5	H	486	ILE
5	H	504	SER
5	H	514	ARG
5	H	515	ASP
5	H	517	GLN
5	H	521	ILE
5	H	533	SER
5	H	541	ILE
5	H	542	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	99	GLN
1	A	100	ASN
1	A	112	GLN
1	A	147	GLN
1	A	150	HIS
1	A	211	ASN
1	A	225	GLN

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Mol	Chain	Res	Type
1	A	280	GLN
1	A	281	ASN
1	A	409	ASN
1	A	455	GLN
1	A	534	GLN
2	B	211	ASN
2	B	242	ASN
2	B	356	GLN
2	B	435	GLN
2	B	455	GLN
2	B	534	GLN
2	B	543	ASN
1	C	65	ASN
1	C	112	GLN
1	C	147	GLN
1	C	211	ASN
1	C	281	ASN
1	C	298	HIS
1	C	356	GLN
1	C	409	ASN
1	C	423	ASN
1	C	455	GLN
1	D	15	ASN
1	D	211	ASN
1	D	225	GLN
1	D	268	GLN
1	D	271	ASN
1	D	281	ASN
1	D	356	GLN
1	D	385	ASN
1	D	435	GLN
1	D	455	GLN
1	D	534	GLN
3	E	147	GLN
3	E	149	HIS
3	E	280	GLN
3	E	281	ASN
3	E	356	GLN
3	E	435	GLN
3	E	455	GLN
3	E	525	GLN
1	F	15	ASN

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Mol	Chain	Res	Type
1	F	65	ASN
1	F	99	GLN
1	F	211	ASN
1	F	281	ASN
1	F	312	ASN
1	F	356	GLN
1	F	409	ASN
1	F	435	GLN
1	F	455	GLN
4	G	242	ASN
4	G	268	GLN
4	G	281	ASN
4	G	298	HIS
4	G	356	GLN
4	G	509	GLN
4	G	534	GLN
5	H	99	GLN
5	H	175	ASN
5	H	211	ASN
5	H	225	GLN
5	H	281	ASN
5	H	298	HIS
5	H	356	GLN
5	H	409	ASN
5	H	435	GLN
5	H	455	GLN
5	H	534	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 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	$\# Z > 2$
6	EDO	C	603	-	3,3,3	0.09	0	2,2,2	0.18	0
6	EDO	A	602	-	3,3,3	0.08	0	2,2,2	0.00	0
6	EDO	C	604	-	3,3,3	0.14	0	2,2,2	0.06	0
6	EDO	H	602	-	3,3,3	0.16	0	2,2,2	0.33	0
6	EDO	D	601	-	3,3,3	0.05	0	2,2,2	0.23	0
6	EDO	B	601	-	3,3,3	0.19	0	2,2,2	0.25	0
6	EDO	C	602	-	3,3,3	0.34	0	2,2,2	0.26	0
7	GOL	A	604	-	5,5,5	0.19	0	5,5,5	0.50	0
6	EDO	C	601	-	3,3,3	0.44	0	2,2,2	0.50	0
6	EDO	H	601	-	3,3,3	0.13	0	2,2,2	0.17	0
6	EDO	F	602	-	3,3,3	0.96	0	2,2,2	1.48	0
6	EDO	G	601	-	3,3,3	0.10	0	2,2,2	0.66	0
6	EDO	A	601	-	3,3,3	0.41	0	2,2,2	1.39	0
6	EDO	A	603	-	3,3,3	0.29	0	2,2,2	0.39	0
6	EDO	F	601	-	3,3,3	0.07	0	2,2,2	0.19	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
6	EDO	C	603	-	-	0/1/1/1	-
6	EDO	A	602	-	-	1/1/1/1	-
6	EDO	C	604	-	-	1/1/1/1	-
6	EDO	H	602	-	-	1/1/1/1	-
6	EDO	D	601	-	-	0/1/1/1	-
6	EDO	B	601	-	-	1/1/1/1	-
6	EDO	C	602	-	-	1/1/1/1	-
7	GOL	A	604	-	-	2/4/4/4	-
6	EDO	C	601	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	H	601	-	-	1/1/1/1	-
6	EDO	F	602	-	-	1/1/1/1	-
6	EDO	G	601	-	-	1/1/1/1	-
6	EDO	A	601	-	-	1/1/1/1	-
6	EDO	A	603	-	-	1/1/1/1	-
6	EDO	F	601	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	604	GOL	O1-C1-C2-C3
7	A	604	GOL	O1-C1-C2-O2
6	F	602	EDO	O1-C1-C2-O2
6	G	601	EDO	O1-C1-C2-O2
6	A	601	EDO	O1-C1-C2-O2
6	A	602	EDO	O1-C1-C2-O2
6	A	603	EDO	O1-C1-C2-O2
6	B	601	EDO	O1-C1-C2-O2
6	C	602	EDO	O1-C1-C2-O2
6	F	601	EDO	O1-C1-C2-O2
6	H	602	EDO	O1-C1-C2-O2
6	C	604	EDO	O1-C1-C2-O2
6	H	601	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	601	EDO	1	0
7	A	604	GOL	2	0
6	G	601	EDO	1	0

5.7 Other polymers [i](#)

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	546/553 (98%)	-1.10	1 (0%) 91 91	44, 78, 129, 185	0
1	C	553/553 (100%)	-1.07	2 (0%) 88 87	29, 77, 141, 196	0
1	D	553/553 (100%)	-1.09	3 (0%) 87 85	25, 80, 147, 220	0
1	F	553/553 (100%)	-1.05	3 (0%) 87 85	46, 84, 156, 239	0
2	B	504/528 (95%)	-0.98	1 (0%) 91 91	38, 94, 167, 236	0
3	E	534/548 (97%)	-0.99	1 (0%) 91 91	50, 86, 162, 206	0
4	G	504/526 (95%)	-0.77	8 (1%) 70 64	37, 83, 208, 271	0
5	H	543/553 (98%)	-1.04	0 100 100	48, 87, 169, 235	0
All	All	4290/4367 (98%)	-1.02	19 (0%) 88 87	25, 83, 166, 271	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	267	GLY	11.1
4	G	208	VAL	4.4
1	A	142	PHE	3.9
1	F	142	PHE	3.8
1	F	14	PHE	3.0
1	C	142	PHE	2.6
1	C	518	TYR	2.6
1	D	197	HIS	2.6
1	D	144	PRO	2.6
1	F	13	GLY	2.4
4	G	290	VAL	2.4
3	E	16	GLY	2.3
4	G	264	HIS	2.3
2	B	142	PHE	2.3
1	D	518	TYR	2.2
4	G	216	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
4	G	263	LEU	2.1
4	G	260	LEU	2.0
4	G	291	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	C	603	4/4	0.94	0.14	88,99,109,110	0
6	EDO	B	601	4/4	0.96	0.11	56,64,68,79	0
6	EDO	A	602	4/4	0.96	0.11	85,92,94,95	0
6	EDO	F	601	4/4	0.96	0.10	94,106,106,113	0
6	EDO	D	601	4/4	0.97	0.10	89,91,92,103	0
6	EDO	A	603	4/4	0.97	0.11	69,75,84,88	0
6	EDO	H	602	4/4	0.97	0.08	68,84,84,89	0
6	EDO	H	601	4/4	0.98	0.14	89,94,105,105	0
6	EDO	C	604	4/4	0.98	0.12	80,82,86,90	0
7	GOL	A	604	6/6	0.98	0.05	87,99,99,109	0
8	MN	B	602	1/1	0.98	0.03	141,141,141,141	1
8	MN	F	604	1/1	0.98	0.04	91,91,91,91	1
6	EDO	C	602	4/4	0.99	0.04	58,60,67,72	0
6	EDO	A	601	4/4	0.99	0.06	33,37,38,42	0
8	MN	A	605	1/1	0.99	0.04	133,133,133,133	1
6	EDO	G	601	4/4	0.99	0.05	60,68,71,71	0
8	MN	C	606	1/1	0.99	0.02	129,129,129,129	1
8	MN	D	603	1/1	0.99	0.02	164,164,164,164	1
8	MN	D	604	1/1	0.99	0.04	113,113,113,113	1
8	MN	E	601	1/1	0.99	0.03	117,117,117,117	1

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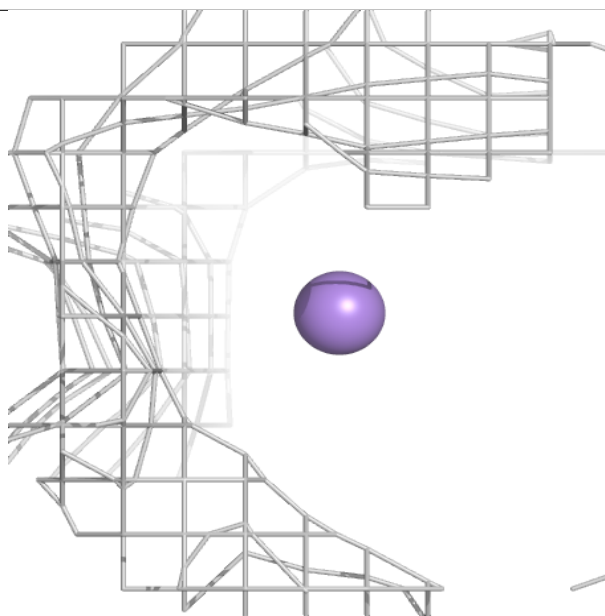
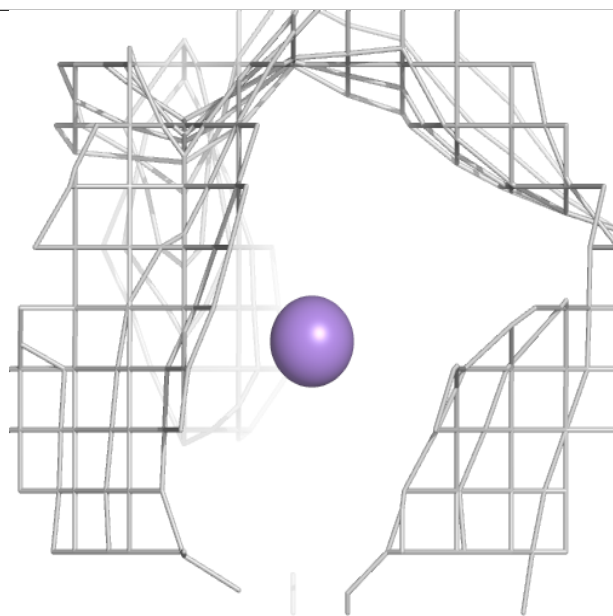
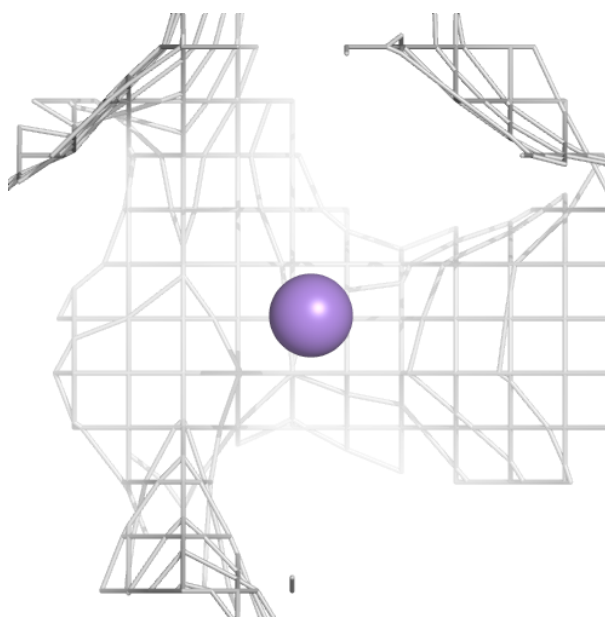
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	C	601	4/4	0.99	0.07	67,78,83,84	0
8	MN	H	603	1/1	0.99	0.02	111,111,111,111	1
9	CL	C	605	1/1	0.99	0.04	76,76,76,76	0
9	CL	D	602	1/1	0.99	0.04	73,73,73,73	0
8	MN	F	603	1/1	1.00	0.04	127,127,127,127	1
6	EDO	F	602	4/4	1.00	0.06	21,29,30,31	0
8	MN	G	602	1/1	1.00	0.02	106,106,106,106	1

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

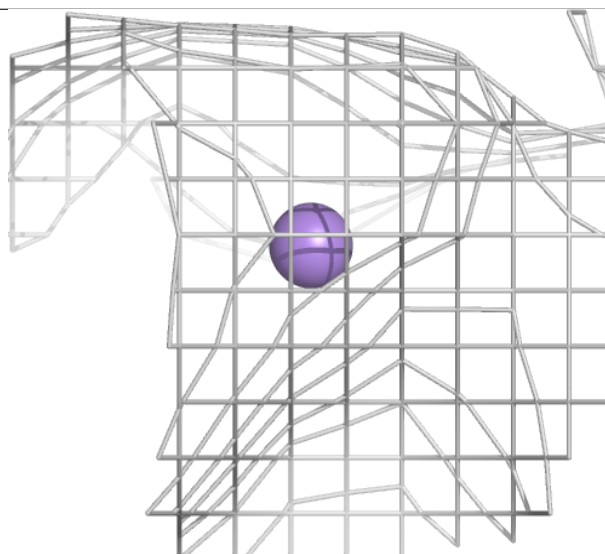
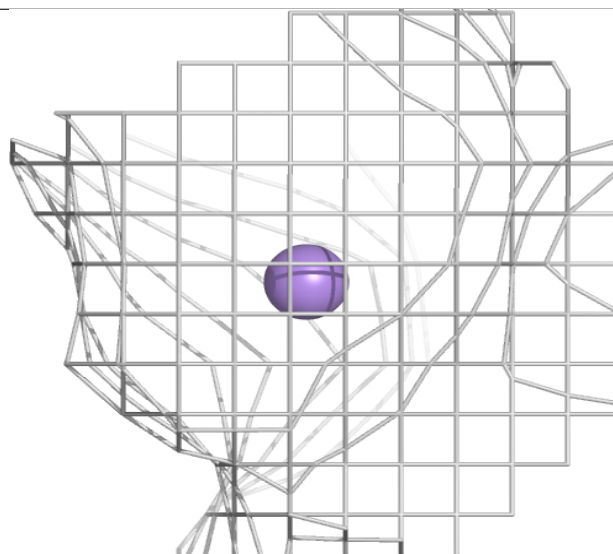
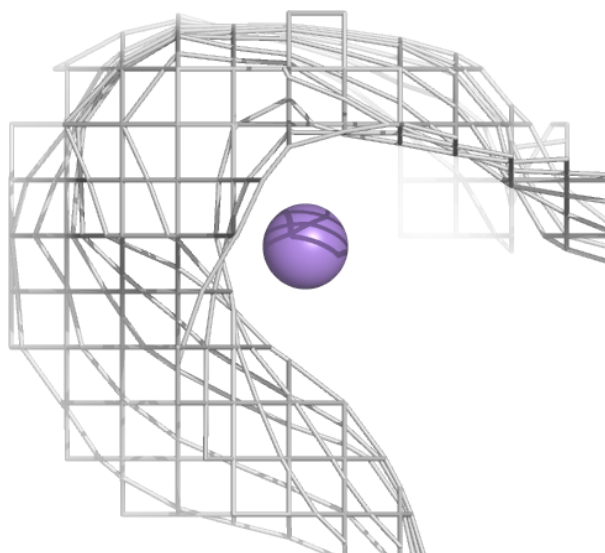
Electron density around MN B 602:

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



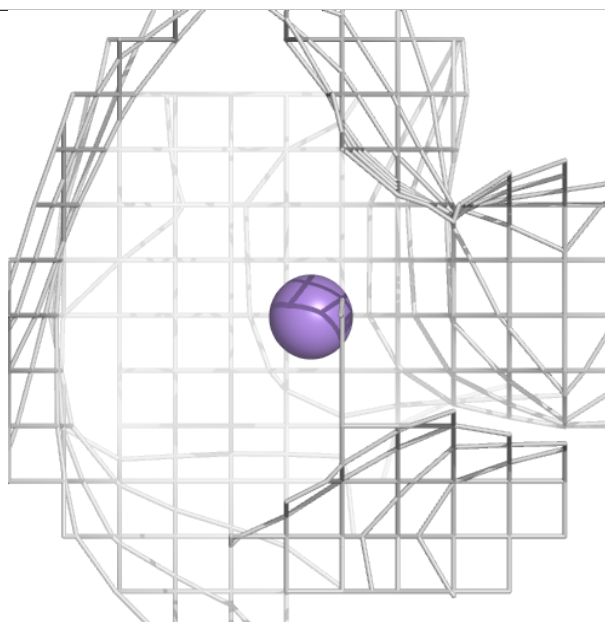
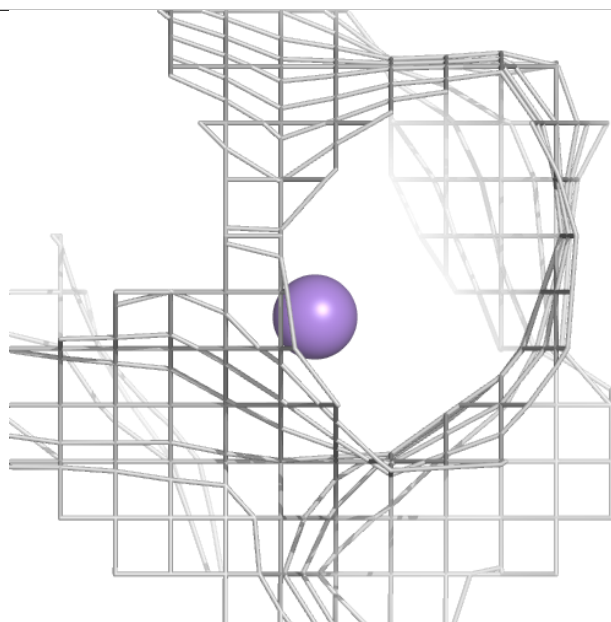
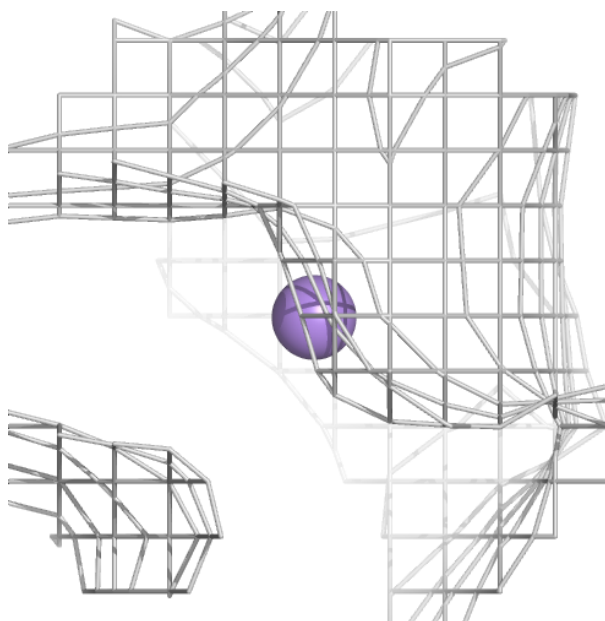
Electron density around MN F 604:

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



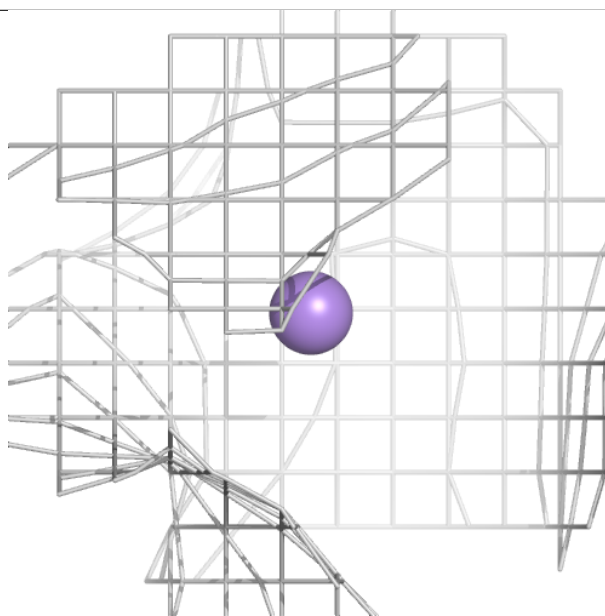
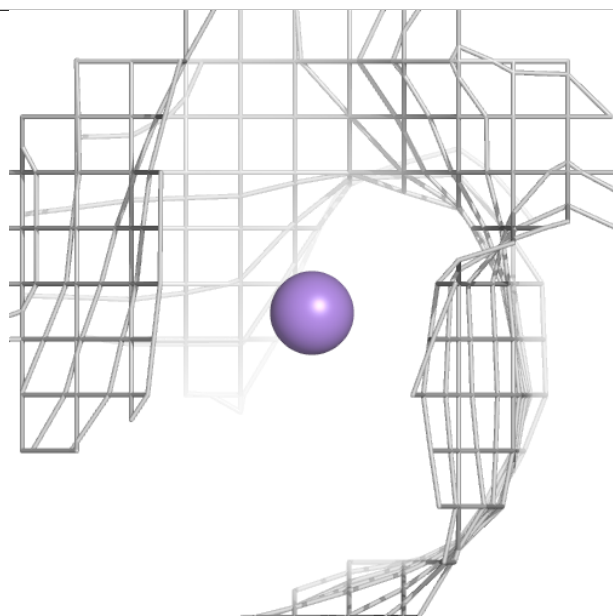
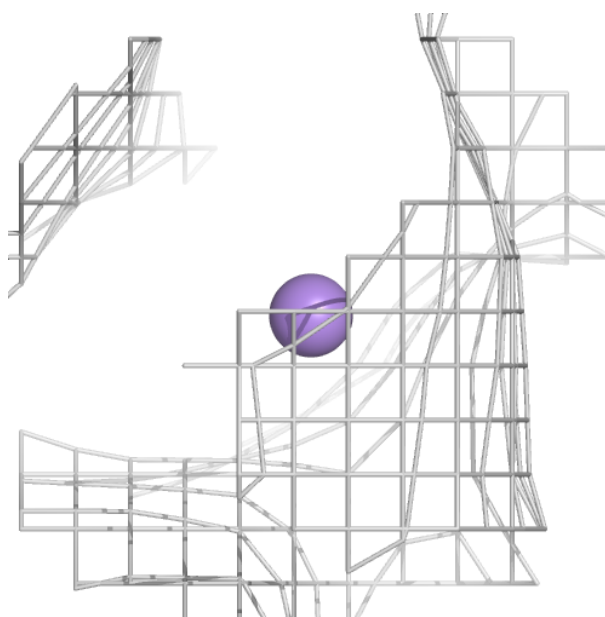
Electron density around MN A 605:

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



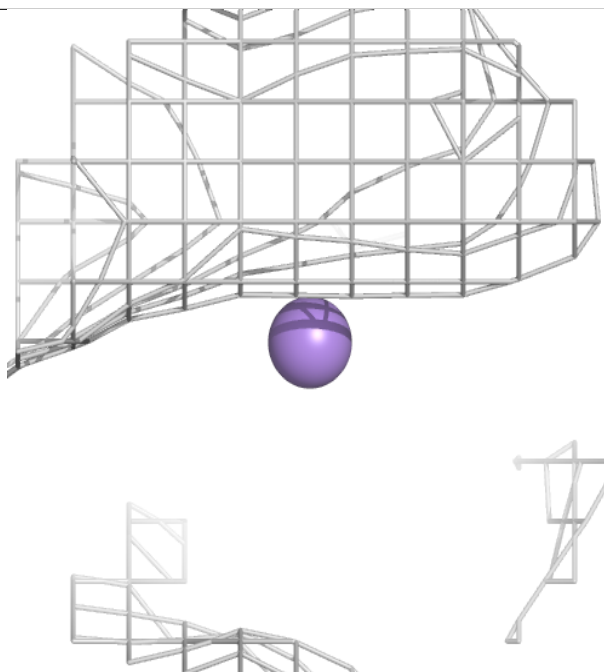
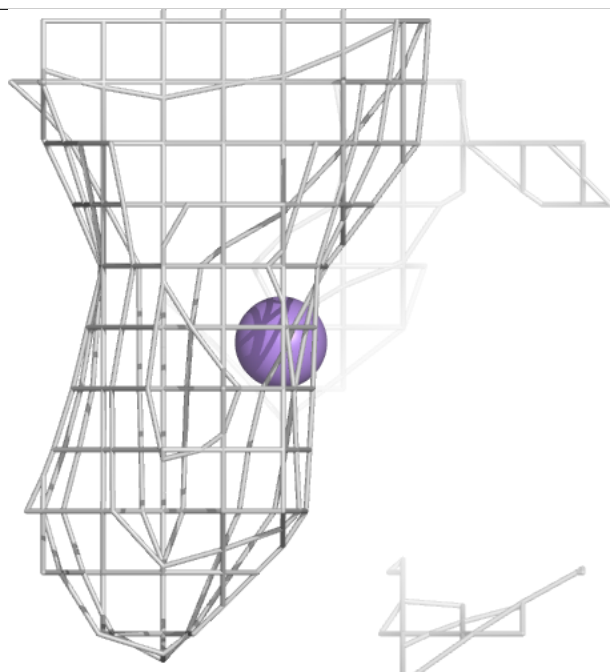
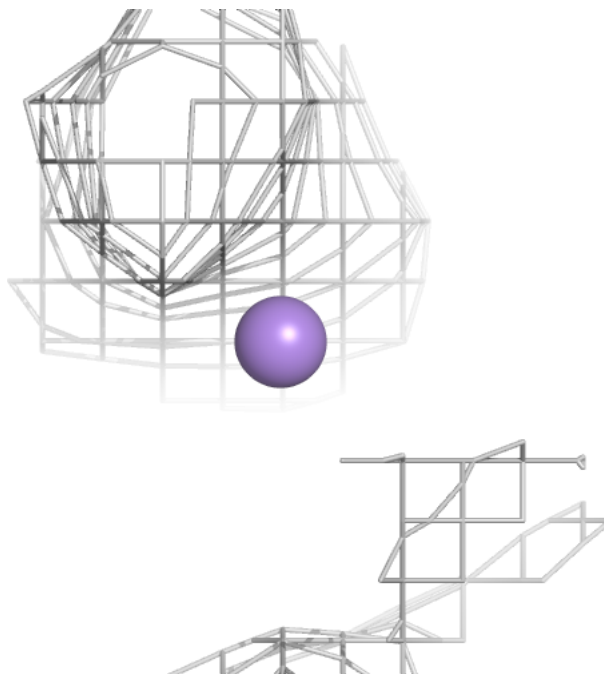
Electron density around MN C 606:

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



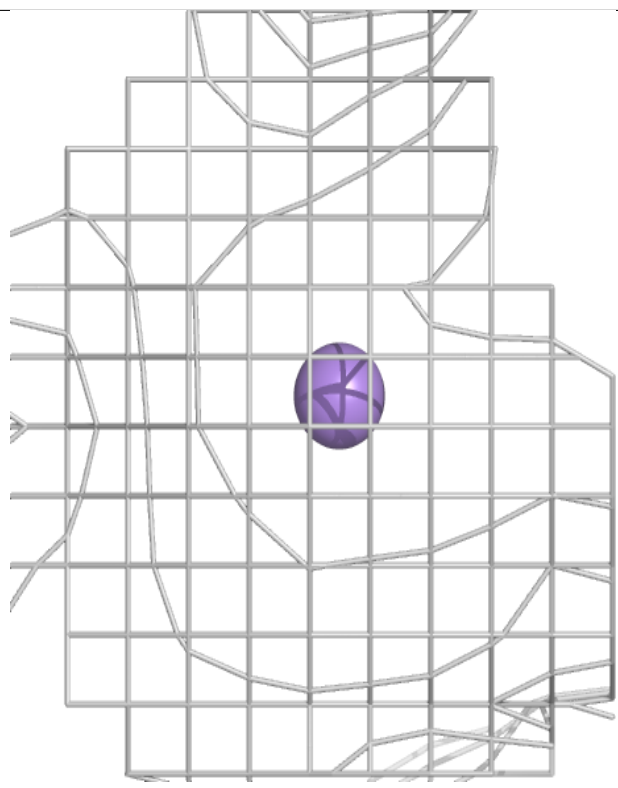
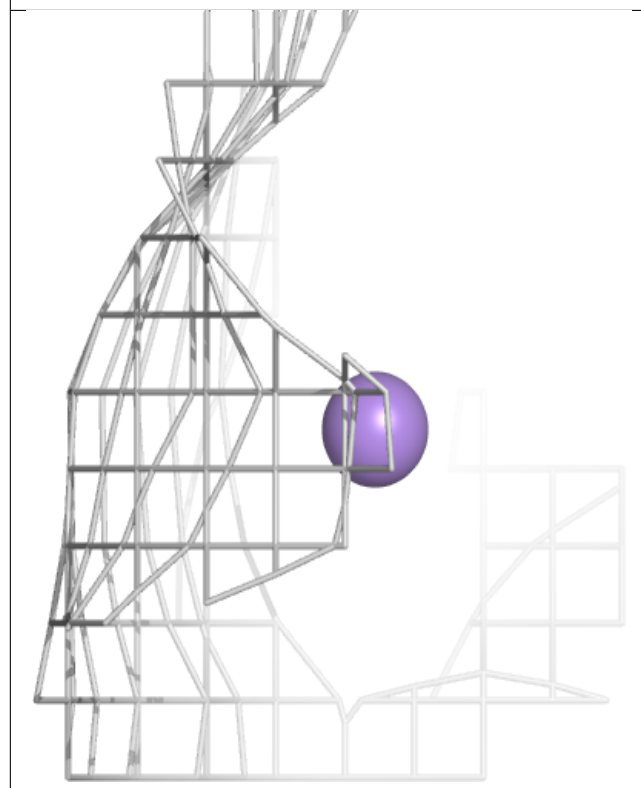
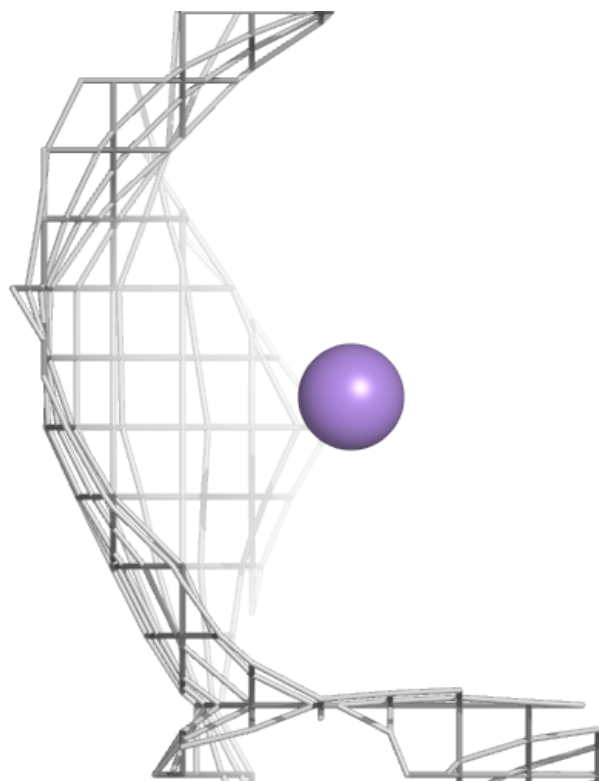
Electron density around MN D 603:

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



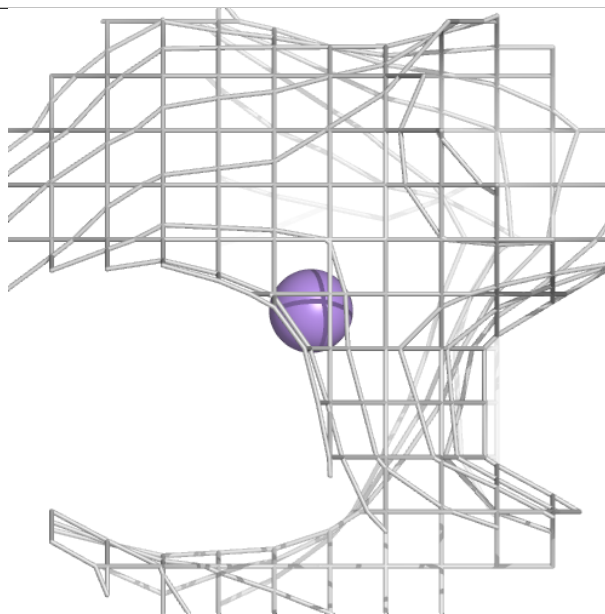
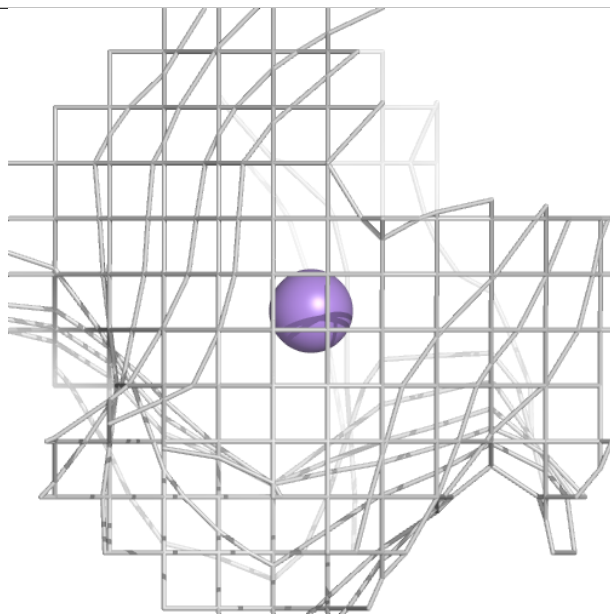
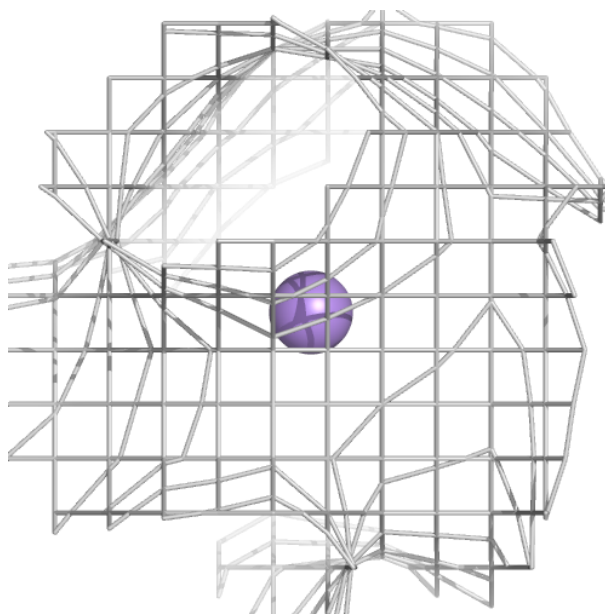
Electron density around MN D 604:

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



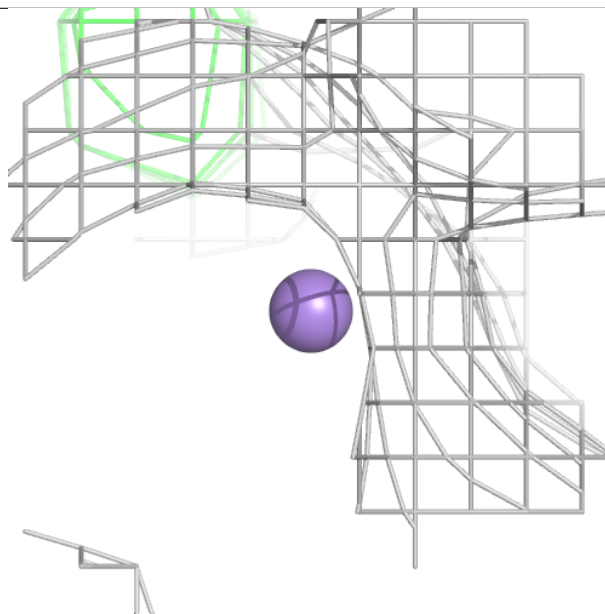
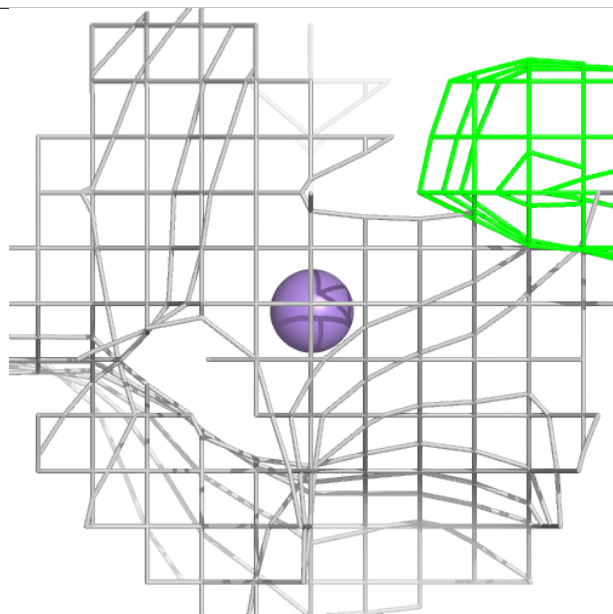
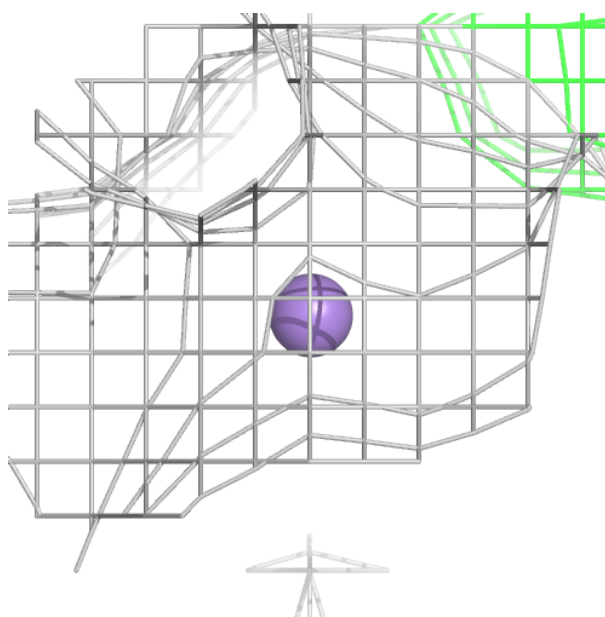
Electron density around MN E 601:

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



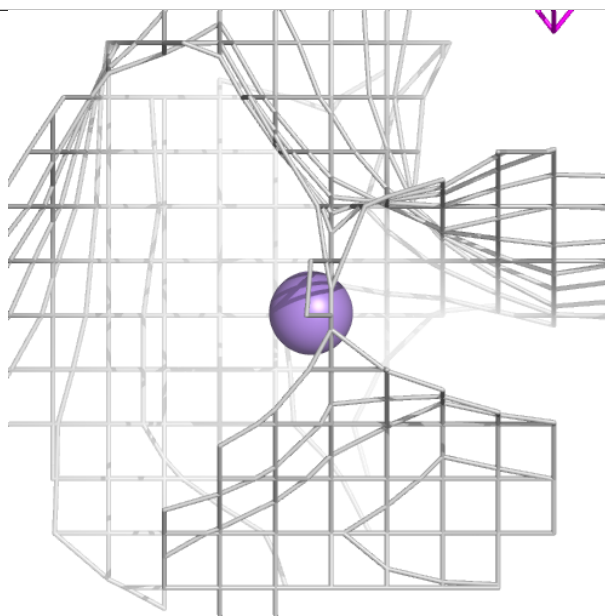
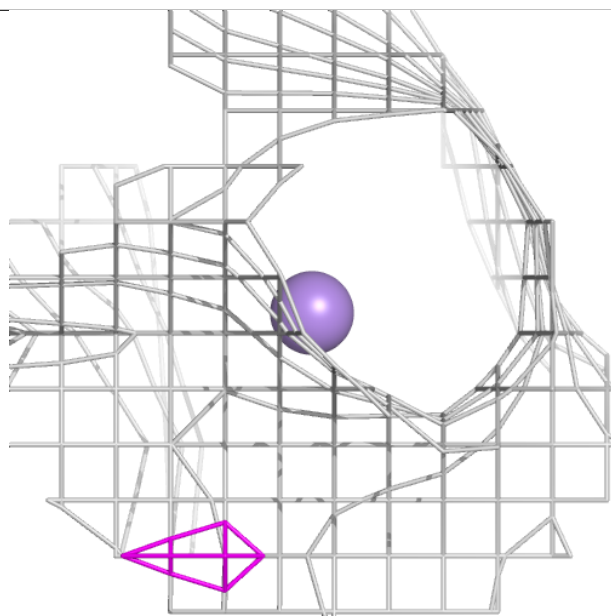
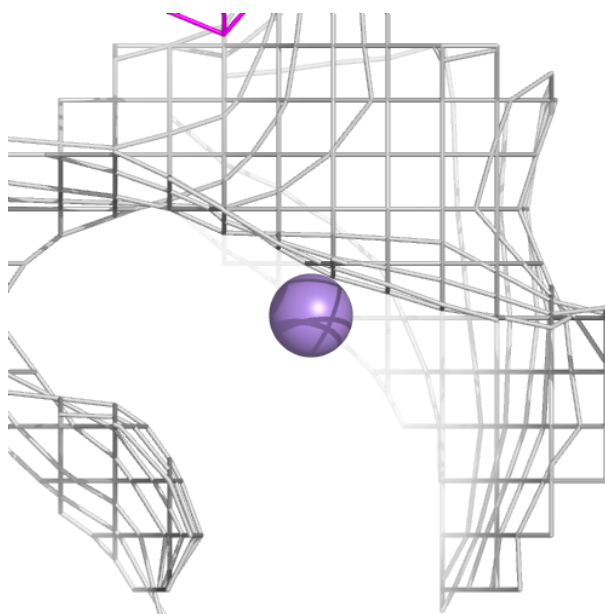
Electron density around MN H 603:

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



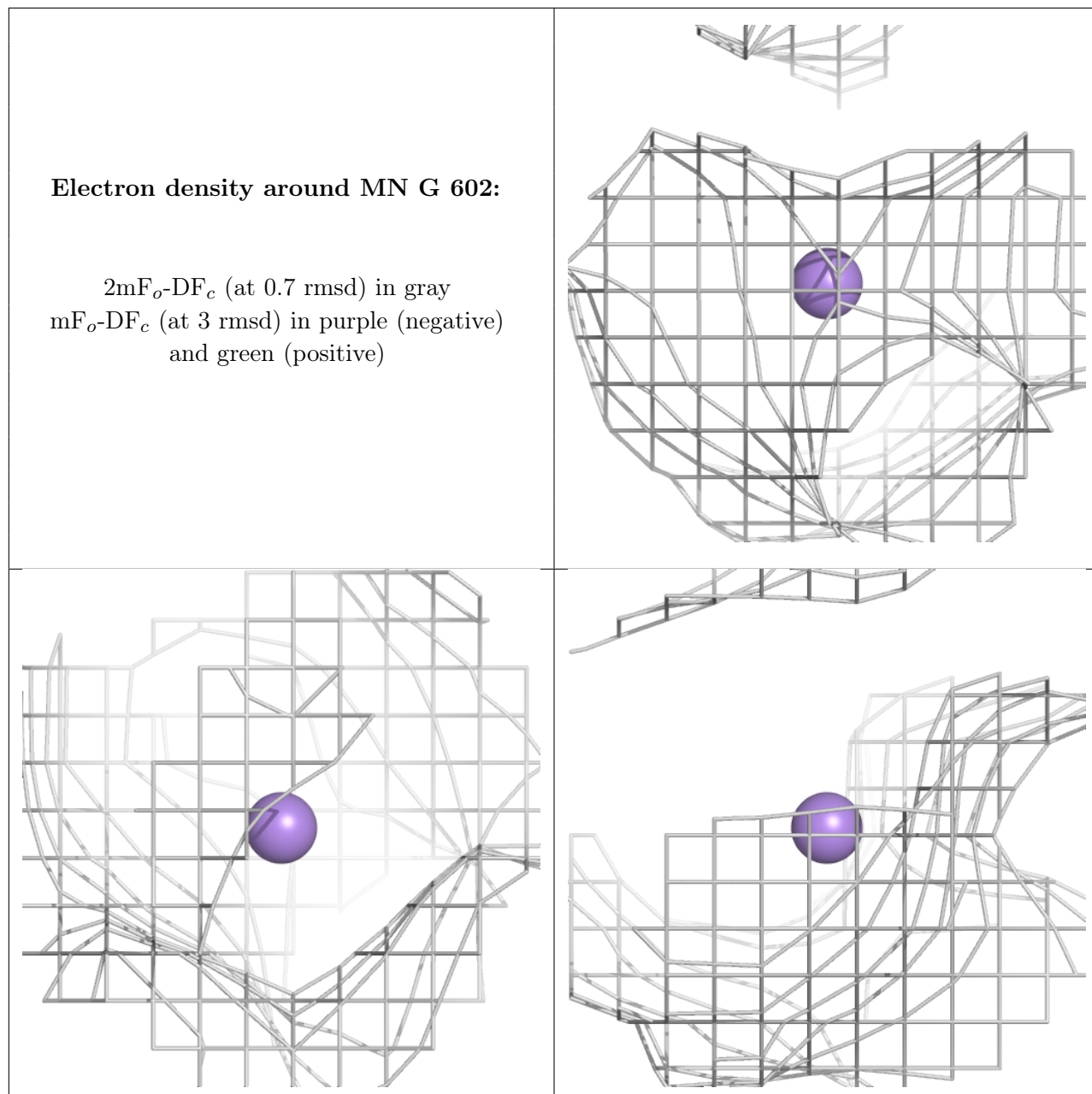
Electron density around MN F 603:

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



Electron density around MN G 602:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.