



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:40 AM UTC

PDB ID : 2BDI / pdb_00002bdi
Title : Human Kallikrein 4 complex with cobalt and p-aminobenzamidine
Authors : Debela, M.; Bode, W.; Goettig, P.; Structural Proteomics in Europe (SPINE)
Deposited on : 2005-10-20
Resolution : 3.00 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

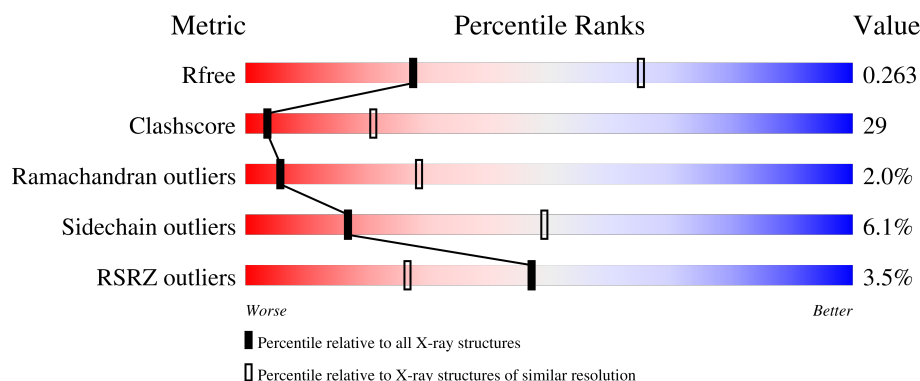
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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	223	4% 43% 47% 10%
1	B	223	2% 44% 48% 8%
1	C	223	3% 48% 41% 10%
1	D	223	4% 48% 43% 9%
1	E	223	4% 45% 44% 10%

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Mol	Chain	Length	Quality of chain
1	F	223	
1	G	223	
1	H	223	
1	I	223	
1	J	223	
1	K	223	
1	L	223	
1	M	223	
1	N	223	
1	O	223	
1	P	223	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PBZ	A	701	-	X	-	-
3	PBZ	D	704	-	-	X	-
3	PBZ	L	712	-	X	-	-
3	PBZ	O	715	-	X	X	-
3	PBZ	P	716	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27340 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.

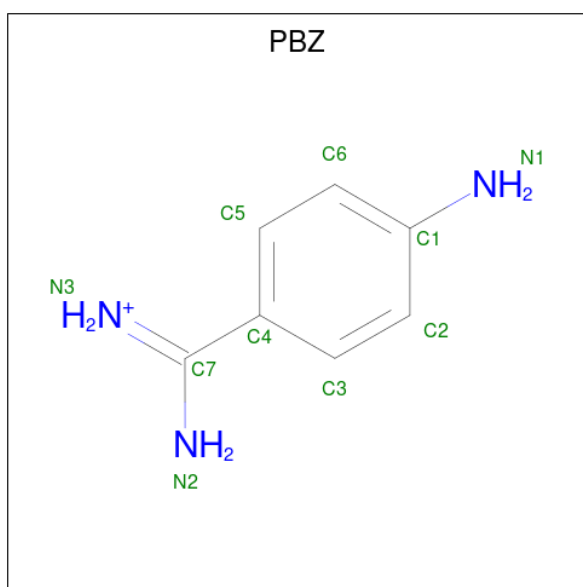
- Molecule 1 is a protein called Kallikrein-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	135	0	0
			1670	1043	281	329	17			
1	B	223	Total	C	N	O	S	80	0	0
			1670	1043	281	329	17			
1	C	223	Total	C	N	O	S	62	0	0
			1670	1043	281	329	17			
1	D	223	Total	C	N	O	S	91	0	0
			1670	1043	281	329	17			
1	E	223	Total	C	N	O	S	90	0	0
			1670	1043	281	329	17			
1	F	223	Total	C	N	O	S	54	0	0
			1670	1043	281	329	17			
1	G	223	Total	C	N	O	S	81	0	0
			1670	1043	281	329	17			
1	H	223	Total	C	N	O	S	120	0	0
			1670	1043	281	329	17			
1	I	223	Total	C	N	O	S	105	0	0
			1670	1043	281	329	17			
1	J	223	Total	C	N	O	S	56	0	0
			1670	1043	281	329	17			
1	K	223	Total	C	N	O	S	78	0	0
			1670	1043	281	329	17			
1	L	223	Total	C	N	O	S	73	0	0
			1670	1043	281	329	17			
1	M	223	Total	C	N	O	S	48	0	0
			1670	1043	281	329	17			
1	N	223	Total	C	N	O	S	63	0	0
			1670	1043	281	329	17			
1	O	223	Total	C	N	O	S	67	0	0
			1670	1043	281	329	17			
1	P	223	Total	C	N	O	S	86	0	0
			1670	1043	281	329	17			

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		
2	E	1	Total	Co	0	0
			1	1		
2	I	1	Total	Co	0	0
			1	1		
2	M	1	Total	Co	0	0
			1	1		

- Molecule 3 is P-AMINO BENZAMIDINE (CCD ID: PBZ) (formula: C₇H₁₀N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	7	3		
3	B	1	Total	C	N	0	0
			10	7	3		
3	C	1	Total	C	N	0	0
			10	7	3		
3	D	1	Total	C	N	0	0
			10	7	3		
3	E	1	Total	C	N	0	0
			10	7	3		
3	F	1	Total	C	N	0	0
			10	7	3		
3	G	1	Total	C	N	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	N	0	0
			10	7	3		
3	I	1	Total	C	N	0	0
			10	7	3		
3	J	1	Total	C	N	0	0
			10	7	3		
3	K	1	Total	C	N	0	0
			10	7	3		
3	L	1	Total	C	N	0	0
			10	7	3		
3	M	1	Total	C	N	0	0
			10	7	3		
3	N	1	Total	C	N	0	0
			10	7	3		
3	O	1	Total	C	N	0	0
			10	7	3		
3	P	1	Total	C	N	0	0
			10	7	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	27	Total	O	0	0
			27	27		
4	C	30	Total	O	0	0
			30	30		
4	D	37	Total	O	0	0
			37	37		
4	E	26	Total	O	0	0
			26	26		
4	F	36	Total	O	0	0
			36	36		
4	G	25	Total	O	0	0
			25	25		
4	H	21	Total	O	0	0
			21	21		
4	I	20	Total	O	0	0
			20	20		
4	J	22	Total	O	0	0
			22	22		

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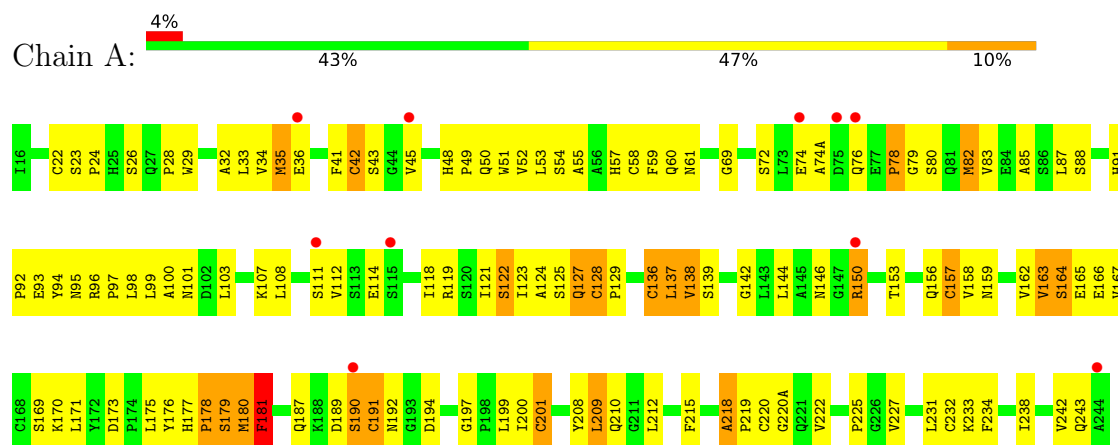
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	21	Total 21	O 21	0	0
4	L	39	Total 39	O 39	0	0
4	M	37	Total 37	O 37	0	0
4	N	29	Total 29	O 29	0	0
4	O	28	Total 28	O 28	0	0
4	P	32	Total 32	O 32	0	0

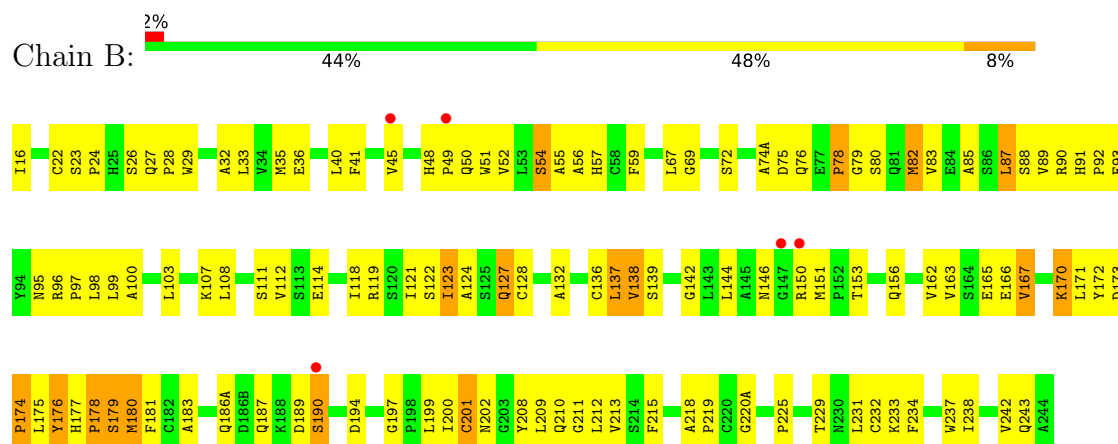
3 Residue-property plots [i](#)

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.

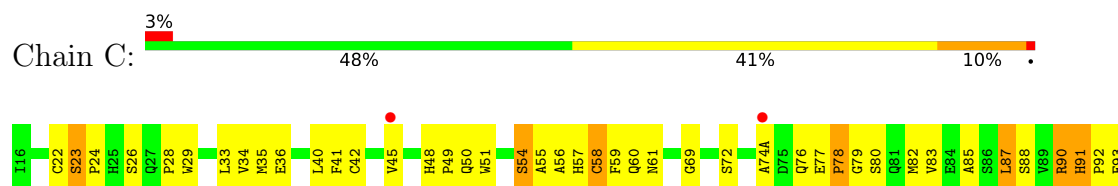
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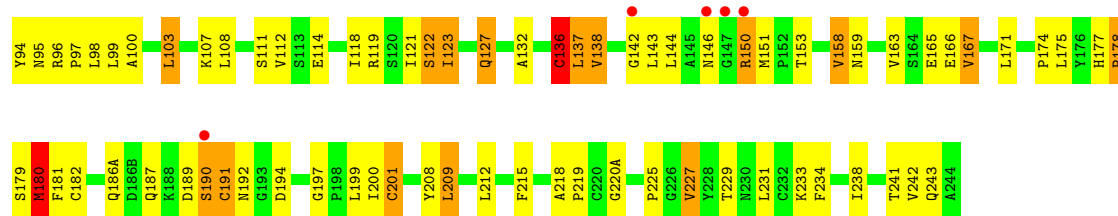


• Molecule 1: Kallikrein-4

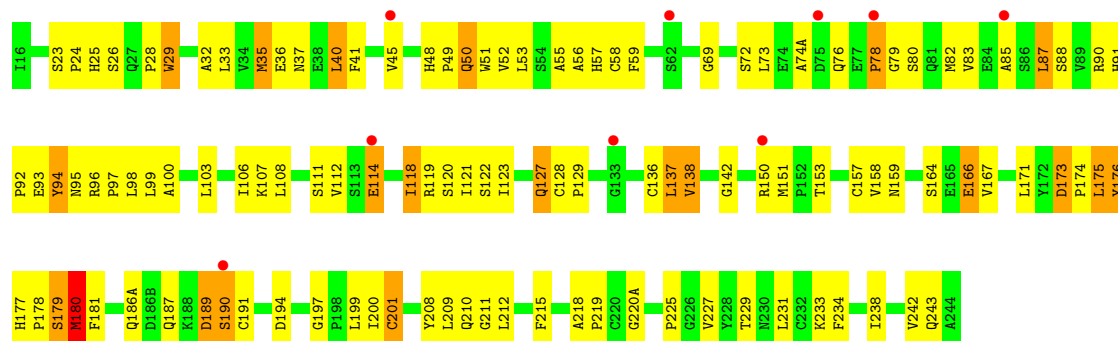


• Molecule 1: Kallikrein-4

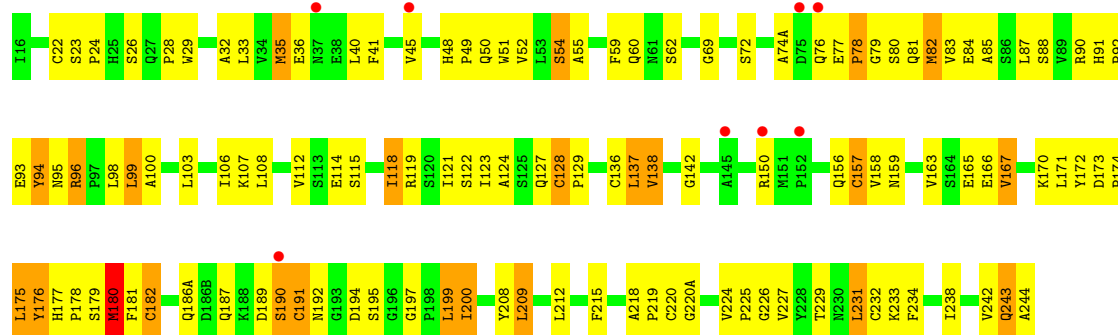
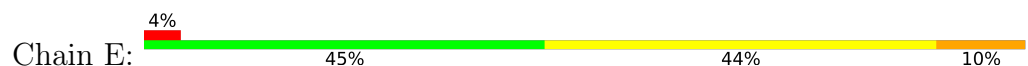




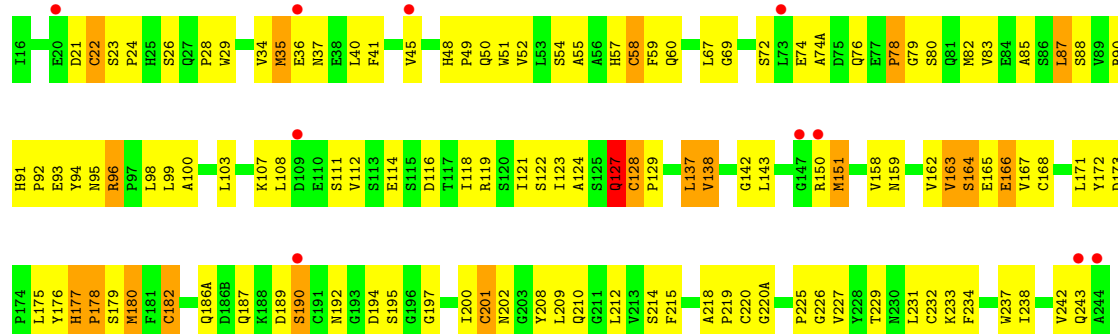
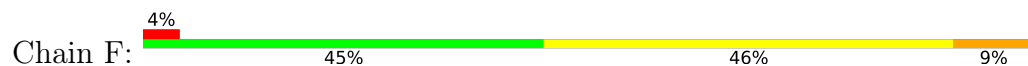
• Molecule 1: Kallikrein-4



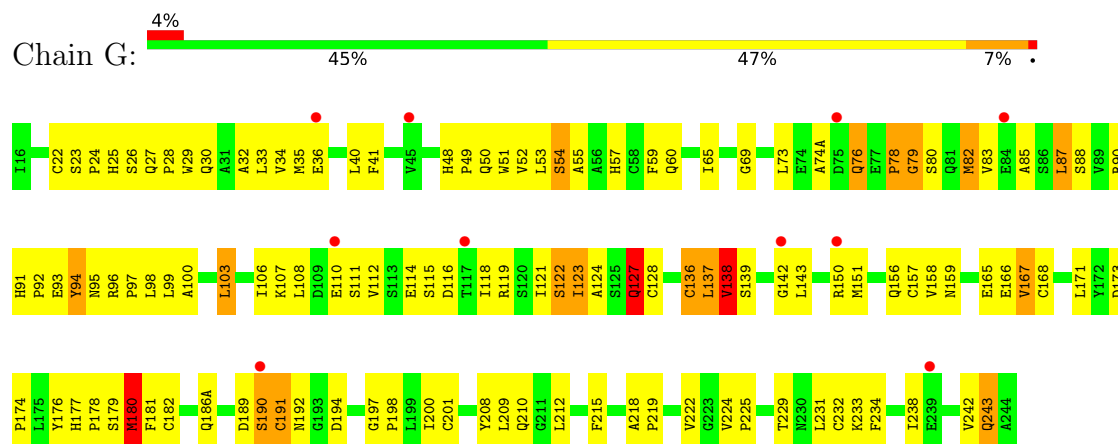
• Molecule 1: Kallikrein-4



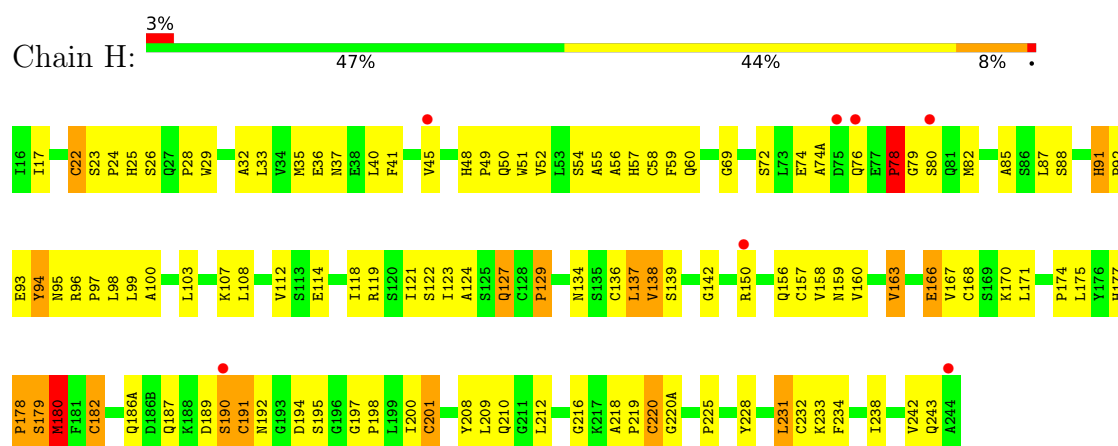
• Molecule 1: Kallikrein-4



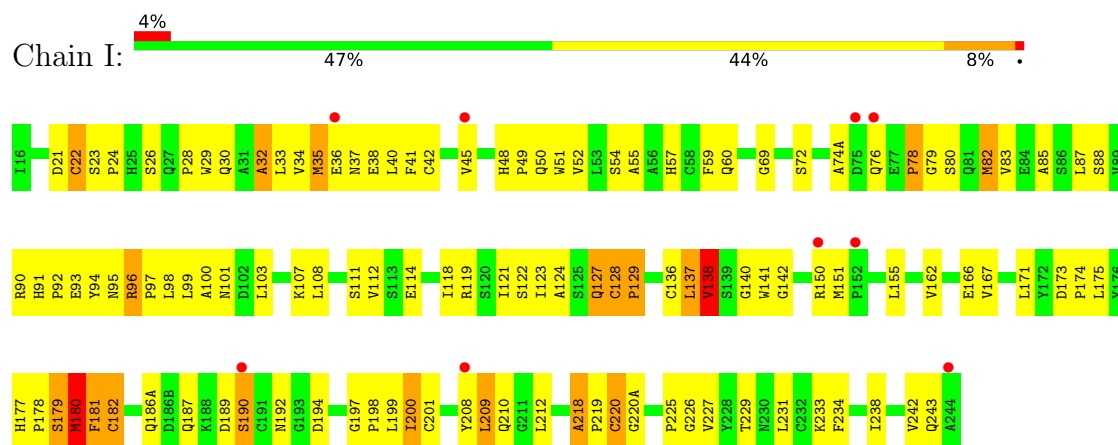
- Molecule 1: Kallikrein-4



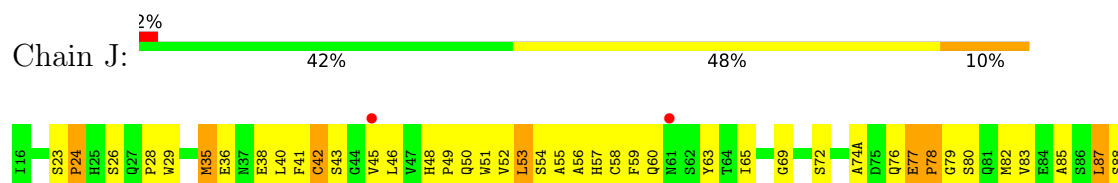
- Molecule 1: Kallikrein-4

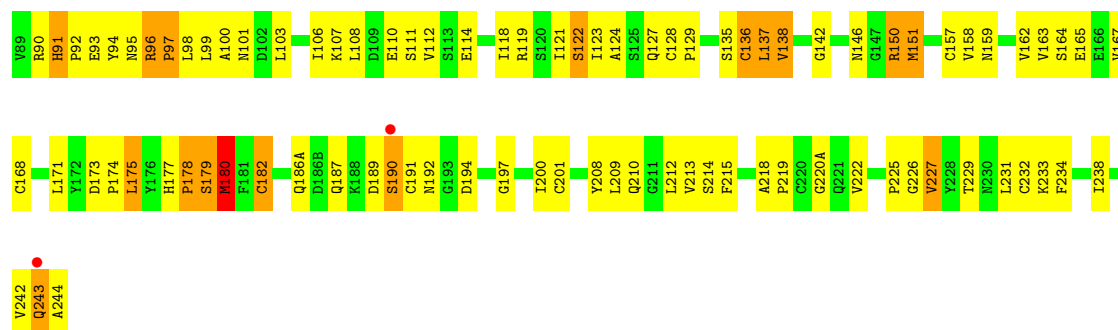


- Molecule 1: Kallikrein-4

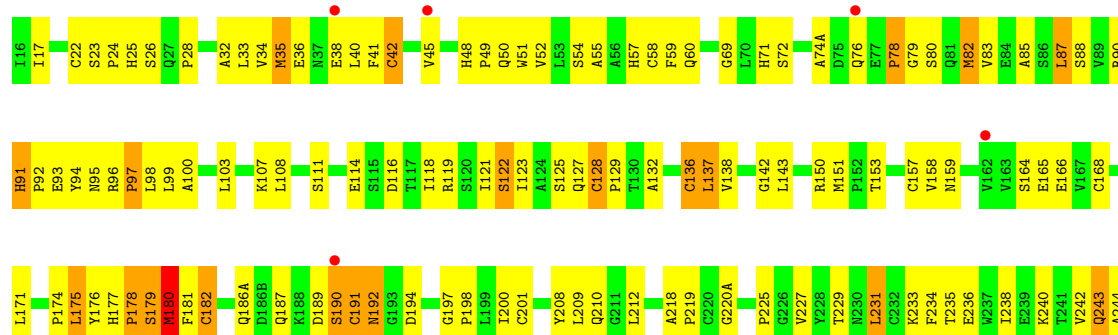
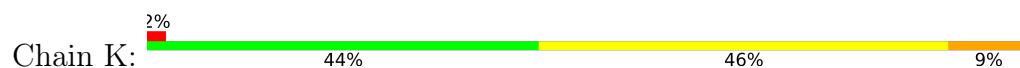


- Molecule 1: Kallikrein-4

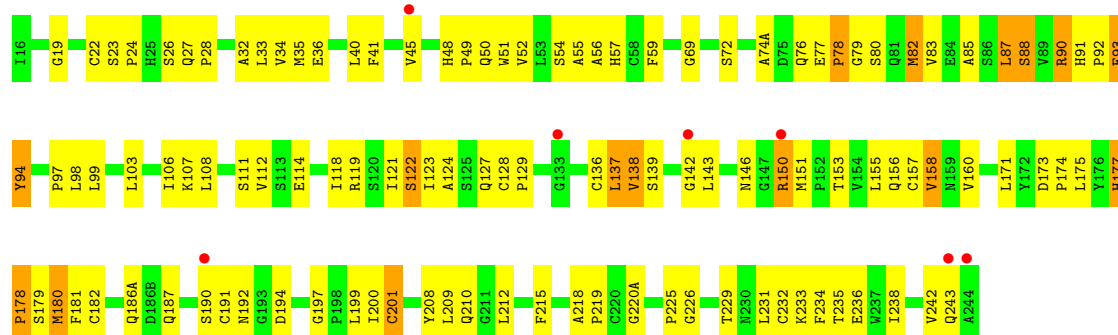




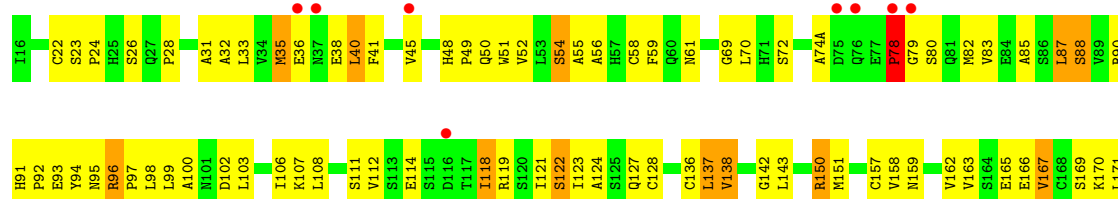
• Molecule 1: Kallikrein-4

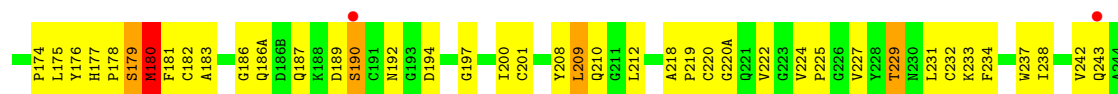


• Molecule 1: Kallikrein-4

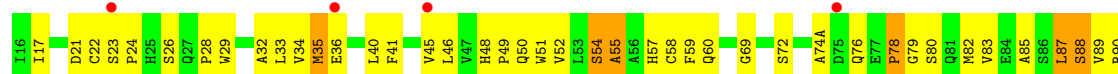
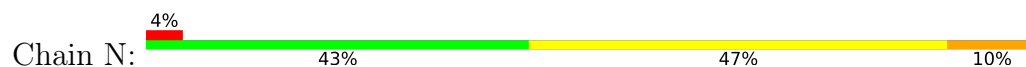


• Molecule 1: Kallikrein-4

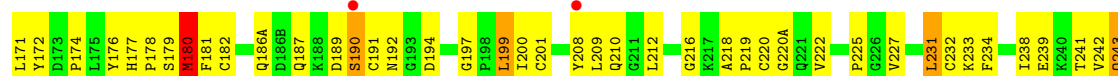
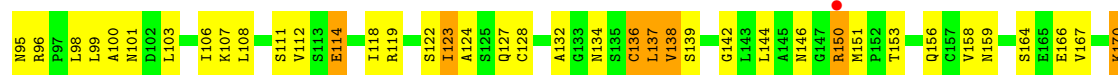
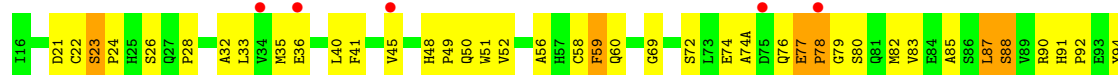




• Molecule 1: Kallikrein-4

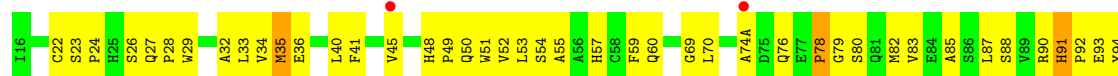


• Molecule 1: Kallikrein-4



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• Molecule 1: Kallikrein-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	147.05Å 73.86Å 154.38Å 90.00° 102.41° 90.00°	Depositor
Resolution (Å)	19.90 – 3.00 19.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.90-3.00) 96.2 (19.90-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.258 , 0.296 0.259 , 0.263	Depositor DCC
R_{free} test set	3199 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	27340	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 46.08 % 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 1.2048e-04. 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: PBZ, CO

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	1.73	20/1707 (1.2%)	1.40	10/2323 (0.4%)
1	B	1.74	26/1707 (1.5%)	1.38	6/2323 (0.3%)
1	C	1.68	20/1707 (1.2%)	1.38	10/2323 (0.4%)
1	D	1.76	26/1707 (1.5%)	1.38	7/2323 (0.3%)
1	E	1.77	27/1707 (1.6%)	1.40	12/2323 (0.5%)
1	F	1.88	26/1707 (1.5%)	1.39	12/2323 (0.5%)
1	G	1.79	24/1707 (1.4%)	1.41	12/2323 (0.5%)
1	H	1.72	23/1707 (1.3%)	1.43	14/2323 (0.6%)
1	I	1.70	21/1707 (1.2%)	1.39	8/2323 (0.3%)
1	J	1.75	29/1707 (1.7%)	1.39	10/2323 (0.4%)
1	K	1.71	27/1707 (1.6%)	1.39	9/2323 (0.4%)
1	L	1.69	19/1707 (1.1%)	1.34	3/2323 (0.1%)
1	M	1.84	27/1707 (1.6%)	1.37	8/2323 (0.3%)
1	N	1.80	28/1707 (1.6%)	1.40	14/2323 (0.6%)
1	O	1.70	25/1707 (1.5%)	1.36	12/2323 (0.5%)
1	P	1.76	28/1707 (1.6%)	1.40	11/2323 (0.5%)
All	All	1.75	396/27312 (1.4%)	1.39	158/37168 (0.4%)

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	B	0	1
1	G	0	1
1	I	0	1
1	K	0	1
1	N	0	1
1	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	7

All (396) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	22	CYS	CA-C	12.87	1.69	1.52
1	L	201	CYS	CA-C	-11.14	1.41	1.53
1	G	180	MET	SD-CE	-9.48	1.55	1.79
1	C	191	CYS	C-O	-9.05	1.12	1.23
1	G	168	CYS	C-O	-9.04	1.13	1.24
1	G	52	VAL	CA-CB	-8.99	1.43	1.54
1	J	77	GLU	C-O	-8.97	1.17	1.25
1	D	106	ILE	CA-CB	-8.78	1.43	1.54
1	K	157	CYS	C-N	-8.76	1.28	1.33
1	F	201	CYS	CA-CB	8.65	1.65	1.52
1	P	180	MET	SD-CE	-8.63	1.57	1.79
1	P	136	CYS	C-O	-8.56	1.12	1.23
1	F	163	VAL	CA-CB	-8.52	1.43	1.54
1	A	163	VAL	CA-CB	-8.48	1.43	1.54
1	I	22	CYS	CA-C	8.42	1.63	1.52
1	J	136	CYS	C-O	8.38	1.33	1.24
1	M	96	ARG	N-CA	-8.36	1.38	1.46
1	J	52	VAL	CA-CB	-8.29	1.44	1.54
1	B	124	ALA	CA-CB	-8.26	1.40	1.53
1	D	94	TYR	C-O	-8.23	1.13	1.23
1	C	136	CYS	CA-CB	-8.20	1.41	1.53
1	F	173	ASP	CA-C	8.18	1.61	1.53
1	L	177	HIS	N-CA	8.18	1.52	1.45
1	P	52	VAL	CA-CB	-8.15	1.44	1.54
1	E	176	TYR	C-O	-8.08	1.14	1.23
1	D	180	MET	CG-SD	8.06	2.00	1.80
1	H	94	TYR	C-O	-8.06	1.14	1.23
1	B	52	VAL	CA-CB	-8.04	1.44	1.54
1	M	182	CYS	CA-C	-7.97	1.43	1.52
1	F	220	CYS	CA-C	-7.92	1.41	1.53
1	A	191	CYS	CA-C	7.87	1.63	1.52
1	K	191	CYS	CA-C	7.87	1.62	1.52
1	F	128	CYS	CA-C	-7.82	1.43	1.53
1	B	237	TRP	C-O	-7.74	1.15	1.24
1	F	35	MET	CA-C	-7.71	1.44	1.53
1	L	52	VAL	CA-CB	-7.68	1.44	1.54
1	G	222	VAL	C-O	-7.66	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	220	CYS	C-O	-7.65	1.13	1.23
1	N	182	CYS	C-O	-7.60	1.14	1.23
1	G	151	MET	SD-CE	7.59	1.98	1.79
1	O	136	CYS	CA-C	-7.53	1.43	1.52
1	E	35	MET	CA-C	-7.52	1.45	1.53
1	K	82	MET	SD-CE	7.50	1.98	1.79
1	F	58	CYS	CA-C	7.48	1.62	1.52
1	E	94	TYR	C-O	-7.42	1.15	1.23
1	K	180	MET	SD-CE	-7.36	1.61	1.79
1	M	181	PHE	CA-C	-7.33	1.43	1.52
1	N	128	CYS	CA-CB	-7.31	1.40	1.53
1	O	128	CYS	C-O	-7.30	1.14	1.23
1	F	128	CYS	C-O	-7.28	1.14	1.24
1	H	22	CYS	CA-C	7.27	1.62	1.53
1	N	52	VAL	CA-CB	-7.26	1.45	1.54
1	P	96	ARG	C-O	7.26	1.31	1.24
1	B	162	VAL	CA-CB	-7.24	1.46	1.54
1	L	191	CYS	C-O	-7.23	1.17	1.24
1	N	132	ALA	C-O	-7.15	1.15	1.23
1	F	52	VAL	CA-CB	-7.13	1.45	1.54
1	H	134	ASN	C-O	-7.13	1.15	1.23
1	N	128	CYS	CA-C	-7.12	1.44	1.53
1	E	199	LEU	N-CA	-7.11	1.38	1.46
1	O	222	VAL	C-O	-7.08	1.16	1.24
1	C	158	VAL	CA-CB	-7.05	1.50	1.55
1	F	124	ALA	CA-CB	-6.99	1.42	1.53
1	O	114	GLU	C-O	-6.96	1.15	1.24
1	G	180	MET	CG-SD	6.96	1.98	1.80
1	I	127	GLN	CA-C	6.95	1.62	1.52
1	A	52	VAL	CA-CB	-6.94	1.45	1.54
1	G	136	CYS	CA-C	-6.93	1.44	1.52
1	G	22	CYS	C-O	6.93	1.32	1.23
1	B	173	ASP	CA-C	6.92	1.60	1.53
1	O	182	CYS	CA-C	-6.87	1.44	1.52
1	N	136	CYS	C-O	6.86	1.32	1.23
1	M	222	VAL	CA-CB	6.86	1.61	1.54
1	P	160	VAL	C-O	-6.86	1.17	1.23
1	F	168	CYS	CA-C	6.85	1.61	1.52
1	I	82	MET	SD-CE	6.83	1.96	1.79
1	E	128	CYS	C-O	-6.79	1.14	1.23
1	C	42	CYS	CA-C	-6.77	1.44	1.53
1	I	162	VAL	CA-CB	-6.72	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	52	VAL	CA-CB	-6.69	1.46	1.54
1	J	173	ASP	CA-C	6.67	1.59	1.53
1	D	201	CYS	CA-C	-6.66	1.45	1.52
1	G	173	ASP	CA-C	6.65	1.59	1.53
1	L	151	MET	SD-CE	6.64	1.96	1.79
1	J	91	HIS	CA-C	6.64	1.60	1.53
1	J	124	ALA	CA-CB	-6.64	1.42	1.53
1	P	136	CYS	CA-C	-6.64	1.44	1.52
1	J	35	MET	CA-C	-6.63	1.46	1.53
1	M	106	ILE	CA-CB	-6.63	1.46	1.54
1	M	52	VAL	CA-CB	-6.61	1.46	1.54
1	M	170	LYS	C-O	-6.60	1.16	1.24
1	A	173	ASP	CA-C	6.58	1.59	1.53
1	I	35	MET	CA-C	-6.58	1.46	1.53
1	H	201	CYS	CA-C	-6.56	1.44	1.52
1	P	201	CYS	N-CA	-6.52	1.38	1.46
1	F	195	SER	CA-C	-6.49	1.44	1.52
1	N	173	ASP	CA-C	6.47	1.59	1.53
1	N	231	LEU	CA-C	-6.46	1.43	1.52
1	A	162	VAL	CA-CB	-6.46	1.47	1.54
1	M	180	MET	SD-CE	-6.44	1.63	1.79
1	O	106	ILE	CA-CB	-6.42	1.46	1.54
1	K	231	LEU	C-O	-6.42	1.16	1.24
1	C	103	LEU	CA-C	6.39	1.60	1.52
1	L	34	VAL	CA-CB	-6.38	1.46	1.54
1	P	201	CYS	C-O	6.37	1.31	1.23
1	B	211	GLY	C-O	6.36	1.30	1.23
1	D	180	MET	SD-CE	-6.36	1.63	1.79
1	L	124	ALA	CA-CB	-6.35	1.42	1.53
1	A	124	ALA	CA-CB	-6.34	1.42	1.53
1	J	151	MET	SD-CE	6.32	1.95	1.79
1	G	82	MET	SD-CE	6.30	1.95	1.79
1	B	127	GLN	CA-C	6.29	1.61	1.53
1	F	96	ARG	N-CA	-6.28	1.40	1.46
1	P	189	ASP	C-O	-6.28	1.17	1.23
1	J	213	VAL	CA-CB	-6.27	1.46	1.54
1	B	151	MET	SD-CE	6.27	1.95	1.79
1	D	127	GLN	CA-C	6.26	1.61	1.52
1	P	170	LYS	C-O	-6.24	1.16	1.24
1	O	180	MET	SD-CE	-6.22	1.64	1.79
1	N	58	CYS	N-CA	6.22	1.53	1.46
1	E	118	ILE	C-O	-6.21	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	151	MET	SD-CE	6.20	1.95	1.79
1	O	164	SER	CA-C	-6.20	1.44	1.52
1	M	52	VAL	C-O	-6.18	1.17	1.24
1	M	35	MET	CA-C	-6.18	1.46	1.53
1	H	179	SER	CA-C	-6.17	1.42	1.52
1	O	132	ALA	CA-CB	-6.17	1.43	1.53
1	P	127	GLN	CA-C	6.16	1.61	1.52
1	A	136	CYS	C-O	6.14	1.32	1.23
1	J	180	MET	SD-CE	-6.14	1.64	1.79
1	P	181	PHE	CA-C	-6.14	1.45	1.52
1	J	164	SER	CA-C	-6.13	1.44	1.52
1	E	175	LEU	C-O	-6.13	1.16	1.24
1	E	180	MET	CG-SD	6.13	1.96	1.80
1	I	52	VAL	CA-CB	-6.13	1.46	1.54
1	B	170	LYS	CA-C	-6.12	1.44	1.52
1	J	162	VAL	C-O	-6.10	1.17	1.24
1	M	31	ALA	C-O	-6.09	1.16	1.24
1	H	124	ALA	CA-CB	-6.09	1.43	1.53
1	C	97	PRO	CA-C	-6.08	1.40	1.52
1	H	97	PRO	CA-C	-6.07	1.40	1.52
1	K	136	CYS	CA-CB	-6.04	1.45	1.53
1	N	181	PHE	CA-C	-6.04	1.45	1.52
1	A	218	ALA	CA-C	-6.04	1.46	1.52
1	F	127	GLN	CA-C	6.03	1.61	1.53
1	H	166	GLU	CA-CB	-6.02	1.44	1.53
1	C	34	VAL	CA-CB	-6.01	1.46	1.54
1	B	213	VAL	CA-CB	-6.00	1.46	1.54
1	K	42	CYS	C-O	6.00	1.31	1.23
1	J	65	ILE	CA-CB	-5.99	1.46	1.54
1	G	167	VAL	CA-CB	-5.99	1.47	1.54
1	N	163	VAL	CA-CB	-5.98	1.46	1.54
1	P	35	MET	CA-C	-5.98	1.46	1.53
1	G	124	ALA	CA-CB	-5.97	1.43	1.53
1	E	106	ILE	CA-CB	-5.96	1.47	1.54
1	K	151	MET	SD-CE	5.95	1.94	1.79
1	O	134	ASN	C-O	-5.94	1.16	1.23
1	N	218	ALA	CA-C	-5.94	1.46	1.52
1	O	52	VAL	CA-CB	-5.94	1.47	1.54
1	K	182	CYS	C-O	5.94	1.31	1.23
1	E	82	MET	SD-CE	5.93	1.94	1.79
1	H	232	CYS	C-O	5.93	1.31	1.24
1	D	191	CYS	CA-CB	5.92	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	96	ARG	N-CA	-5.92	1.41	1.46
1	N	176	TYR	C-O	-5.91	1.16	1.23
1	I	180	MET	SD-CE	-5.88	1.64	1.79
1	B	27	GLN	C-O	-5.88	1.17	1.24
1	J	167	VAL	CA-CB	-5.88	1.47	1.54
1	N	55	ALA	CA-C	-5.87	1.45	1.52
1	H	170	LYS	C-O	-5.87	1.16	1.24
1	M	229	THR	C-O	-5.86	1.17	1.23
1	D	118	ILE	C-O	-5.85	1.17	1.24
1	D	164	SER	CA-C	-5.85	1.45	1.52
1	K	175	LEU	N-CA	-5.85	1.38	1.46
1	N	96	ARG	N-CA	-5.85	1.41	1.46
1	F	166	GLU	CA-C	-5.84	1.45	1.52
1	E	182	CYS	CA-C	-5.84	1.45	1.52
1	I	180	MET	CG-SD	5.84	1.95	1.80
1	N	96	ARG	CA-CB	-5.83	1.47	1.53
1	P	201	CYS	CA-C	-5.83	1.45	1.52
1	O	132	ALA	C-O	-5.82	1.17	1.23
1	A	179	SER	CA-C	-5.82	1.43	1.52
1	J	168	CYS	CA-C	-5.81	1.45	1.52
1	P	103	LEU	C-O	5.81	1.31	1.23
1	M	227	VAL	CA-C	5.80	1.59	1.52
1	N	103	LEU	CA-C	5.80	1.59	1.52
1	D	97	PRO	CA-C	-5.80	1.41	1.52
1	P	168	CYS	C-N	-5.80	1.25	1.33
1	E	173	ASP	CA-C	5.79	1.59	1.53
1	H	228	TYR	C-O	5.79	1.31	1.23
1	E	180	MET	SD-CE	-5.79	1.65	1.79
1	L	106	ILE	CA-CB	-5.79	1.47	1.54
1	C	180	MET	SD-CE	-5.78	1.65	1.79
1	O	124	ALA	CA-CB	-5.78	1.43	1.53
1	H	160	VAL	C-O	-5.77	1.18	1.23
1	C	227	VAL	CA-CB	-5.76	1.47	1.54
1	D	157	CYS	C-N	-5.76	1.28	1.33
1	P	99	LEU	CA-C	5.75	1.60	1.52
1	I	42	CYS	C-O	-5.75	1.18	1.24
1	M	22	CYS	C-O	-5.74	1.16	1.23
1	E	172	TYR	C-O	-5.73	1.16	1.24
1	J	46	LEU	C-O	-5.73	1.16	1.23
1	P	180	MET	CG-SD	5.72	1.95	1.80
1	L	88	SER	C-O	-5.72	1.16	1.24
1	M	124	ALA	CA-CB	-5.72	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	123	ILE	CA-C	-5.72	1.45	1.52
1	D	175	LEU	C-O	-5.71	1.16	1.24
1	P	191	CYS	C-O	-5.69	1.17	1.23
1	I	173	ASP	CA-C	5.69	1.58	1.53
1	M	31	ALA	CA-CB	-5.69	1.44	1.53
1	M	163	VAL	CA-CB	-5.69	1.47	1.54
1	L	94	TYR	C-O	-5.69	1.17	1.23
1	J	162	VAL	CA-CB	-5.68	1.48	1.54
1	E	224	VAL	CA-CB	-5.67	1.46	1.54
1	J	135	SER	CA-C	-5.66	1.45	1.52
1	H	127	GLN	CA-C	5.65	1.61	1.53
1	L	160	VAL	C-O	-5.65	1.18	1.23
1	N	124	ALA	CA-CB	-5.65	1.43	1.53
1	E	191	CYS	CA-C	5.64	1.59	1.53
1	N	88	SER	C-O	-5.64	1.16	1.24
1	N	46	LEU	C-O	-5.63	1.17	1.23
1	P	162	VAL	C-O	-5.63	1.17	1.24
1	A	169	SER	N-CA	-5.62	1.39	1.46
1	C	163	VAL	CA-C	5.62	1.59	1.52
1	L	93	GLU	CD-OE1	5.62	1.36	1.25
1	A	157	CYS	C-O	5.61	1.30	1.23
1	P	34	VAL	CA-CB	-5.60	1.47	1.54
1	N	21	ASP	C-O	-5.60	1.17	1.24
1	B	172	TYR	CA-C	-5.59	1.45	1.52
1	P	106	ILE	CA-CB	-5.59	1.47	1.54
1	I	21	ASP	CA-C	-5.59	1.45	1.52
1	K	236	GLU	C-O	-5.58	1.17	1.24
1	N	151	MET	SD-CE	5.58	1.93	1.79
1	A	164	SER	CA-C	-5.58	1.45	1.52
1	F	177	HIS	C-O	-5.58	1.19	1.24
1	F	167	VAL	C-N	5.57	1.40	1.33
1	L	160	VAL	CA-C	-5.57	1.46	1.52
1	K	235	THR	CA-C	5.57	1.59	1.52
1	H	163	VAL	CA-CB	-5.56	1.47	1.54
1	I	218	ALA	CA-C	-5.56	1.45	1.52
1	K	58	CYS	CA-C	-5.56	1.45	1.52
1	O	172	TYR	CA-C	-5.56	1.45	1.52
1	N	35	MET	CA-C	-5.54	1.47	1.53
1	A	58	CYS	CA-C	5.54	1.60	1.52
1	K	181	PHE	CA-C	-5.53	1.45	1.52
1	E	163	VAL	CA-CB	-5.52	1.47	1.54
1	E	231	LEU	C-O	-5.52	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	183	ALA	CA-C	-5.51	1.45	1.52
1	B	22	CYS	C-O	-5.51	1.17	1.23
1	D	128	CYS	C-O	-5.50	1.16	1.24
1	J	167	VAL	CB-CG2	-5.49	1.34	1.52
1	G	138	VAL	N-CA	-5.48	1.40	1.46
1	O	96	ARG	CA-C	-5.48	1.46	1.52
1	K	227	VAL	CA-CB	-5.48	1.47	1.54
1	C	167	VAL	CB-CG2	-5.47	1.34	1.52
1	E	167	VAL	CA-CB	-5.46	1.48	1.54
1	K	52	VAL	CA-CB	-5.46	1.47	1.54
1	I	32	ALA	CA-C	5.46	1.59	1.52
1	C	241	THR	CA-C	-5.46	1.46	1.53
1	D	29	TRP	C-O	-5.45	1.16	1.24
1	A	127	GLN	CA-C	5.44	1.60	1.53
1	I	151	MET	SD-CE	5.43	1.93	1.79
1	B	163	VAL	CA-C	5.43	1.59	1.52
1	K	132	ALA	C-O	-5.43	1.17	1.23
1	O	232	CYS	C-O	-5.43	1.17	1.24
1	K	192	ASN	C-O	5.42	1.30	1.23
1	E	99	LEU	C-O	-5.41	1.17	1.24
1	J	24	PRO	C-O	-5.41	1.17	1.24
1	I	124	ALA	CA-CB	-5.40	1.44	1.53
1	E	52	VAL	CA-CB	-5.40	1.47	1.54
1	A	34	VAL	CA-CB	-5.38	1.47	1.54
1	H	198	PRO	C-O	-5.38	1.17	1.23
1	A	42	CYS	CA-C	-5.38	1.46	1.53
1	B	167	VAL	CB-CG2	-5.38	1.34	1.52
1	J	175	LEU	C-O	-5.38	1.17	1.24
1	I	138	VAL	C-O	5.37	1.29	1.23
1	L	97	PRO	CA-C	-5.37	1.42	1.52
1	H	163	VAL	C-O	-5.37	1.16	1.24
1	M	237	TRP	C-O	-5.37	1.18	1.24
1	K	191	CYS	N-CA	-5.37	1.39	1.46
1	M	169	SER	N-CA	-5.37	1.39	1.46
1	M	179	SER	CA-C	-5.37	1.44	1.52
1	I	96	ARG	N-CA	-5.36	1.41	1.46
1	D	50	GLN	CA-C	5.36	1.59	1.52
1	J	96	ARG	C-O	5.36	1.29	1.24
1	F	164	SER	CA-C	-5.35	1.45	1.52
1	O	241	THR	CA-C	-5.35	1.46	1.53
1	O	170	LYS	C-O	-5.34	1.17	1.24
1	K	34	VAL	CA-CB	-5.34	1.46	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	201	CYS	CA-CB	5.34	1.60	1.52
1	K	198	PRO	C-O	-5.33	1.17	1.23
1	D	173	ASP	CA-C	5.33	1.58	1.53
1	P	177	HIS	C-O	-5.33	1.18	1.24
1	M	167	VAL	CB-CG2	-5.33	1.34	1.52
1	G	127	GLN	CA-C	5.32	1.59	1.52
1	I	200	ILE	CA-C	-5.31	1.46	1.52
1	B	201	CYS	N-CA	-5.31	1.40	1.46
1	F	232	CYS	C-O	-5.31	1.17	1.24
1	C	132	ALA	CA-CB	-5.29	1.44	1.53
1	J	182	CYS	CA-C	-5.29	1.45	1.52
1	B	89	VAL	C-O	5.29	1.30	1.24
1	D	176	TYR	CA-C	-5.29	1.46	1.52
1	L	173	ASP	CA-C	5.29	1.58	1.53
1	N	236	GLU	C-O	-5.29	1.17	1.24
1	H	195	SER	CA-C	-5.28	1.46	1.52
1	G	232	CYS	CA-CB	-5.28	1.44	1.53
1	C	58	CYS	CA-C	-5.27	1.45	1.52
1	G	65	ILE	CA-CB	-5.27	1.47	1.54
1	K	137	LEU	N-CA	-5.27	1.39	1.45
1	G	224	VAL	CA-CB	-5.26	1.47	1.54
1	D	53	LEU	CA-C	-5.26	1.46	1.52
1	N	180	MET	SD-CE	-5.26	1.66	1.79
1	P	154	VAL	CA-CB	-5.24	1.47	1.54
1	J	53	LEU	C-O	5.24	1.30	1.23
1	B	172	TYR	C-O	-5.24	1.16	1.24
1	H	180	MET	SD-CE	-5.23	1.66	1.79
1	K	128	CYS	N-CA	5.23	1.53	1.45
1	A	222	VAL	CA-CB	5.23	1.60	1.54
1	C	123	ILE	C-O	-5.22	1.17	1.24
1	E	124	ALA	CA-CB	-5.21	1.44	1.53
1	F	172	TYR	CA-C	-5.21	1.46	1.52
1	M	224	VAL	CA-CB	-5.21	1.47	1.54
1	M	118	ILE	C-O	-5.21	1.17	1.24
1	E	170	LYS	C-O	-5.21	1.17	1.24
1	O	59	PHE	C-O	-5.20	1.17	1.23
1	C	127	GLN	CA-C	5.20	1.60	1.53
1	K	91	HIS	CA-C	5.19	1.58	1.53
1	I	128	CYS	CA-C	5.18	1.59	1.53
1	J	227	VAL	CA-CB	-5.18	1.48	1.54
1	O	128	CYS	CA-C	-5.18	1.46	1.53
1	P	168	CYS	N-CA	-5.18	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	179	SER	CA-C	-5.17	1.44	1.52
1	P	173	ASP	CA-C	5.17	1.58	1.53
1	C	23	SER	CA-C	5.17	1.58	1.52
1	I	182	CYS	CA-C	-5.17	1.46	1.52
1	F	237	TRP	C-O	-5.17	1.18	1.24
1	A	82	MET	SD-CE	5.17	1.92	1.79
1	A	181	PHE	CA-C	-5.16	1.46	1.52
1	F	34	VAL	CA-CB	-5.16	1.47	1.55
1	F	214	SER	C-O	-5.16	1.17	1.23
1	K	179	SER	CA-C	-5.16	1.45	1.52
1	O	199	LEU	N-CA	-5.15	1.40	1.46
1	H	232	CYS	CA-C	5.15	1.59	1.52
1	O	231	LEU	CA-C	-5.15	1.45	1.52
1	G	103	LEU	CA-C	5.15	1.58	1.52
1	H	231	LEU	C-O	-5.15	1.17	1.24
1	G	232	CYS	CA-C	-5.14	1.45	1.52
1	L	82	MET	SD-CE	5.14	1.92	1.79
1	C	90	ARG	C-O	-5.14	1.17	1.23
1	D	166	GLU	CA-CB	-5.14	1.45	1.53
1	B	128	CYS	CA-CB	-5.14	1.45	1.53
1	J	106	ILE	CA-CB	-5.13	1.48	1.54
1	G	123	ILE	CA-C	-5.13	1.46	1.52
1	F	162	VAL	N-CA	-5.13	1.40	1.46
1	F	182	CYS	C-O	5.13	1.29	1.23
1	B	93	GLU	N-CA	5.12	1.52	1.46
1	D	211	GLY	C-O	5.12	1.28	1.23
1	A	35	MET	CA-C	-5.12	1.47	1.53
1	E	156	GLN	CA-C	-5.12	1.46	1.52
1	H	191	CYS	C-O	-5.12	1.18	1.23
1	G	94	TYR	C-O	-5.11	1.17	1.23
1	L	90	ARG	C-O	-5.11	1.17	1.23
1	B	123	ILE	N-CA	-5.10	1.40	1.46
1	N	89	VAL	CA-CB	-5.10	1.47	1.53
1	K	97	PRO	CA-C	-5.09	1.42	1.52
1	D	175	LEU	CA-C	5.09	1.59	1.52
1	G	34	VAL	CA-CB	-5.09	1.47	1.54
1	G	106	ILE	CA-CB	-5.09	1.48	1.54
1	L	236	GLU	C-O	-5.09	1.18	1.24
1	M	102	ASP	C-O	-5.08	1.17	1.24
1	E	157	CYS	C-N	-5.08	1.30	1.33
1	C	127	GLN	C-O	5.08	1.30	1.23
1	K	35	MET	CA-C	-5.08	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189	ASP	C-O	-5.08	1.18	1.23
1	D	129	PRO	C-O	-5.07	1.17	1.24
1	P	103	LEU	N-CA	5.07	1.52	1.45
1	O	88	SER	C-O	-5.07	1.17	1.24
1	B	132	ALA	C-O	-5.07	1.17	1.23
1	E	224	VAL	C-O	-5.06	1.18	1.24
1	L	56	ALA	CA-CB	-5.06	1.44	1.53
1	M	170	LYS	CA-C	-5.05	1.46	1.52
1	N	172	TYR	CA-C	-5.05	1.46	1.52
1	B	82	MET	SD-CE	5.04	1.92	1.79
1	B	179	SER	CA-C	-5.04	1.44	1.52
1	I	34	VAL	CA-CB	-5.04	1.47	1.55
1	J	182	CYS	C-O	-5.03	1.17	1.23
1	D	114	GLU	C-O	-5.03	1.17	1.24
1	J	163	VAL	CA-CB	-5.02	1.48	1.54
1	M	162	VAL	N-CA	-5.02	1.40	1.46
1	B	56	ALA	C-O	-5.02	1.17	1.24
1	N	34	VAL	CA-CB	-5.02	1.47	1.54
1	P	179	SER	CA-C	-5.02	1.44	1.52
1	O	222	VAL	CA-CB	5.01	1.59	1.54
1	H	52	VAL	CA-CB	-5.01	1.47	1.54
1	J	214	SER	CA-C	-5.00	1.49	1.52
1	B	183	ALA	CA-CB	-5.00	1.45	1.53

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	128	CYS	N-CA-C	10.03	123.93	110.08
1	M	128	CYS	CA-C-N	8.79	128.87	119.90
1	M	128	CYS	C-N-CA	8.79	128.87	119.90
1	P	157	CYS	CA-CB-SG	-8.34	95.21	114.40
1	A	76	GLN	N-CA-C	-8.18	102.06	114.16
1	H	76	GLN	N-CA-C	-8.00	102.32	114.16
1	I	76	GLN	N-CA-C	-7.92	102.45	114.16
1	B	232	CYS	N-CA-C	-7.83	103.47	112.87
1	D	76	GLN	N-CA-C	-7.74	102.71	114.16
1	L	76	GLN	N-CA-C	-7.72	102.73	114.16
1	F	22	CYS	N-CA-CB	7.71	121.02	110.38
1	G	22	CYS	CA-CB-SG	-7.71	96.67	114.40
1	D	157	CYS	CA-C-N	-7.70	113.48	122.11
1	D	157	CYS	C-N-CA	-7.70	113.48	122.11
1	C	76	GLN	N-CA-C	-7.63	102.87	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	76	GLN	N-CA-C	-7.61	102.91	114.16
1	G	76	GLN	N-CA-C	-7.59	102.93	114.16
1	E	76	GLN	N-CA-C	-7.57	102.96	114.16
1	E	100	ALA	N-CA-C	7.47	119.60	110.41
1	O	76	GLN	N-CA-C	-7.47	103.10	114.16
1	P	76	GLN	N-CA-C	-7.46	103.11	114.16
1	H	182	CYS	CB-CA-C	-7.46	97.23	109.53
1	N	76	GLN	N-CA-C	-7.35	103.28	114.16
1	A	128	CYS	N-CA-C	7.32	120.40	110.29
1	H	220	CYS	N-CA-C	7.31	120.17	110.53
1	J	232	CYS	N-CA-C	-7.22	104.60	113.19
1	J	76	GLN	N-CA-C	-7.07	103.69	114.16
1	K	76	GLN	N-CA-C	-7.03	103.76	114.16
1	M	22	CYS	CB-CA-C	-7.01	95.68	111.30
1	J	100	ALA	N-CA-C	6.97	119.52	110.53
1	H	232	CYS	CA-C-O	6.91	130.39	120.51
1	G	100	ALA	N-CA-C	6.82	118.80	110.41
1	K	100	ALA	N-CA-C	6.78	118.75	110.41
1	N	35	MET	CB-CA-C	-6.77	105.94	114.40
1	I	100	ALA	N-CA-C	6.72	118.68	110.41
1	B	76	GLN	N-CA-C	-6.71	104.24	114.16
1	E	128	CYS	N-CA-C	6.70	119.10	110.39
1	H	168	CYS	CB-CA-C	6.69	121.47	110.90
1	L	232	CYS	N-CA-C	-6.51	105.33	113.20
1	H	168	CYS	N-CA-CB	-6.50	100.64	110.07
1	C	201	CYS	CB-CA-C	6.48	120.43	111.23
1	I	220	CYS	N-CA-C	6.44	119.24	110.55
1	C	191	CYS	N-CA-C	6.42	118.61	108.79
1	F	100	ALA	N-CA-C	6.41	118.80	110.53
1	C	136	CYS	CB-CA-C	-6.37	99.26	112.44
1	M	35	MET	CB-CA-C	-6.35	106.46	114.40
1	P	168	CYS	N-CA-C	6.23	118.16	111.36
1	A	100	ALA	N-CA-C	6.22	118.55	110.53
1	K	182	CYS	N-CA-C	6.21	120.01	110.20
1	P	128	CYS	CA-C-N	6.21	127.60	119.84
1	P	128	CYS	C-N-CA	6.21	127.60	119.84
1	G	136	CYS	CA-C-N	-6.21	113.07	122.81
1	G	136	CYS	C-N-CA	-6.21	113.07	122.81
1	N	72	SER	N-CA-C	-6.19	100.55	110.14
1	A	22	CYS	CA-CB-SG	6.17	128.59	114.40
1	H	232	CYS	CA-C-N	-6.17	111.59	122.26
1	H	232	CYS	C-N-CA	-6.17	111.59	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	100	ALA	N-CA-C	6.16	117.99	110.41
1	H	91	HIS	CA-C-O	6.16	125.96	119.80
1	J	35	MET	CB-CA-C	-6.13	106.74	114.40
1	C	100	ALA	N-CA-C	6.10	118.40	110.53
1	H	100	ALA	N-CA-C	6.10	117.91	110.41
1	A	58	CYS	CA-C-O	6.06	126.74	119.59
1	M	100	ALA	N-CA-C	6.04	118.33	110.53
1	H	72	SER	N-CA-C	-6.04	100.78	110.14
1	I	128	CYS	N-CA-C	6.03	119.04	110.24
1	K	72	SER	N-CA-C	-6.01	100.82	110.14
1	K	182	CYS	CB-CA-C	-6.01	99.37	109.53
1	N	128	CYS	CA-CB-SG	-6.01	100.58	114.40
1	D	35	MET	CB-CA-C	-6.01	106.89	114.40
1	C	22	CYS	CA-CB-SG	-6.00	100.60	114.40
1	D	72	SER	N-CA-C	-5.99	100.85	110.14
1	I	179	SER	N-CA-C	-5.98	105.90	112.72
1	N	54	SER	N-CA-C	5.93	116.38	108.38
1	E	35	MET	CB-CA-C	-5.92	107.00	114.40
1	A	42	CYS	CA-C-O	-5.92	114.84	121.05
1	F	21	ASP	CA-C-N	-5.85	110.43	121.66
1	F	21	ASP	C-N-CA	-5.85	110.43	121.66
1	B	72	SER	N-CA-C	-5.85	101.08	110.14
1	O	100	ALA	N-CA-C	5.83	117.58	110.41
1	F	166	GLU	CA-C-N	-5.80	113.12	120.60
1	F	166	GLU	C-N-CA	-5.80	113.12	120.60
1	P	35	MET	CB-CA-C	-5.79	107.17	114.40
1	G	168	CYS	O-C-N	-5.76	116.14	122.07
1	F	72	SER	N-CA-C	-5.76	101.22	110.14
1	D	157	CYS	N-CA-C	5.74	118.82	109.24
1	O	128	CYS	CA-C-N	5.73	127.00	119.84
1	O	128	CYS	C-N-CA	5.73	127.00	119.84
1	O	128	CYS	CA-C-O	-5.67	114.80	120.64
1	F	35	MET	CB-CA-C	-5.66	107.32	114.40
1	E	200	ILE	CA-C-N	-5.66	114.03	122.74
1	E	200	ILE	C-N-CA	-5.66	114.03	122.74
1	N	58	CYS	CB-CA-C	-5.65	101.17	110.72
1	G	128	CYS	CA-C-N	5.65	126.90	119.84
1	G	128	CYS	C-N-CA	5.65	126.90	119.84
1	G	136	CYS	N-CA-C	5.64	117.75	109.24
1	B	100	ALA	N-CA-C	5.63	117.79	110.53
1	I	72	SER	N-CA-C	-5.62	101.42	110.14
1	I	209	LEU	N-CA-C	-5.60	100.00	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	54	SER	N-CA-C	5.59	115.93	108.38
1	J	72	SER	N-CA-C	-5.59	101.48	110.14
1	O	72	SER	N-CA-C	-5.57	101.51	110.14
1	A	35	MET	CB-CA-C	-5.55	107.46	114.40
1	P	182	CYS	CA-CB-SG	5.54	127.15	114.40
1	K	164	SER	N-CA-C	5.54	117.88	110.35
1	N	100	ALA	N-CA-C	5.53	117.21	110.41
1	E	72	SER	N-CA-C	-5.52	101.58	110.14
1	L	72	SER	N-CA-C	-5.52	101.18	109.95
1	I	35	MET	CB-CA-C	-5.51	107.51	114.40
1	F	128	CYS	N-CA-C	5.47	117.83	110.29
1	J	97	PRO	N-CD-CG	-5.46	97.25	103.80
1	M	54	SER	N-CA-C	5.42	115.70	108.38
1	A	72	SER	N-CA-C	-5.40	101.77	110.14
1	H	232	CYS	O-C-N	-5.40	115.40	122.59
1	O	95	ASN	N-CA-C	5.36	119.40	112.86
1	O	128	CYS	N-CA-C	5.34	118.04	110.24
1	C	209	LEU	N-CA-C	-5.33	100.41	108.67
1	O	77	GLU	CA-C-N	5.33	126.51	119.84
1	O	77	GLU	C-N-CA	5.33	126.51	119.84
1	D	100	ALA	N-CA-C	5.30	117.37	110.53
1	E	77	GLU	CA-C-N	5.27	126.43	119.84
1	E	77	GLU	C-N-CA	5.27	126.43	119.84
1	H	97	PRO	N-CD-CG	-5.27	97.48	103.80
1	P	191	CYS	N-CA-C	5.27	116.29	108.60
1	N	157	CYS	N-CA-C	5.26	118.03	109.24
1	P	91	HIS	CA-C-O	5.25	125.05	119.80
1	N	128	CYS	CA-C-N	5.25	126.40	119.84
1	N	128	CYS	C-N-CA	5.25	126.40	119.84
1	J	179	SER	N-CA-C	-5.23	107.07	112.93
1	G	22	CYS	CB-CA-C	5.22	118.38	109.72
1	G	191	CYS	CA-CB-SG	-5.21	102.41	114.40
1	B	54	SER	N-CA-C	5.20	115.40	108.38
1	B	173	ASP	N-CA-C	-5.19	103.63	109.60
1	E	209	LEU	N-CA-C	-5.17	100.65	108.67
1	O	231	LEU	N-CA-C	5.15	117.56	111.33
1	C	91	HIS	CA-C-O	5.13	124.93	119.80
1	K	168	CYS	N-CA-C	5.11	116.85	111.28
1	N	136	CYS	CA-C-N	-5.11	114.79	122.81
1	N	136	CYS	C-N-CA	-5.11	114.79	122.81
1	C	72	SER	N-CA-C	-5.09	102.25	110.14
1	J	42	CYS	CB-CA-C	-5.09	107.18	114.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	99	LEU	N-CA-CB	-5.08	108.37	114.17
1	F	128	CYS	CA-CB-SG	-5.08	102.72	114.40
1	E	231	LEU	N-CA-C	5.06	117.46	111.33
1	F	220	CYS	CA-C-O	-5.06	115.75	121.72
1	H	157	CYS	CA-CB-SG	-5.06	102.77	114.40
1	M	209	LEU	N-CA-C	-5.05	100.84	108.67
1	M	72	SER	N-CA-C	-5.05	102.32	110.14
1	K	128	CYS	CA-CB-SG	-5.04	102.81	114.40
1	P	167	VAL	O-C-N	5.04	126.98	121.90
1	A	201	CYS	CB-CA-C	-5.03	103.03	110.62
1	O	23	SER	CA-C-O	5.03	123.33	119.46
1	J	157	CYS	CA-C-N	-5.03	115.92	122.51
1	J	157	CYS	C-N-CA	-5.03	115.92	122.51
1	A	209	LEU	N-CA-C	-5.03	100.88	108.67
1	E	54	SER	N-CA-C	5.02	115.16	108.38
1	C	54	SER	N-CA-C	5.02	115.16	108.38
1	N	22	CYS	N-CA-C	-5.01	103.92	110.53

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	PHE	Sidechain
1	B	176	TYR	Sidechain
1	G	181	PHE	Sidechain
1	I	181	PHE	Sidechain
1	K	176	TYR	Sidechain
1	N	176	TYR	Sidechain
1	P	176	TYR	Sidechain

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	1670	0	1598	97	0
1	B	1670	0	1598	93	3
1	C	1670	0	1598	99	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1670	0	1598	93	0
1	E	1670	0	1600	88	1
1	F	1670	0	1598	94	1
1	G	1670	0	1602	125	1
1	H	1670	0	1598	83	2
1	I	1670	0	1598	90	1
1	J	1670	0	1598	103	0
1	K	1670	0	1598	96	0
1	L	1670	0	1598	90	0
1	M	1670	0	1598	89	0
1	N	1670	0	1600	100	1
1	O	1670	0	1598	90	1
1	P	1670	0	1598	103	0
2	A	1	0	0	0	0
2	E	1	0	0	0	0
2	I	1	0	0	0	0
2	M	1	0	0	0	0
3	A	10	0	10	2	0
3	B	10	0	10	2	0
3	C	10	0	10	0	0
3	D	10	0	10	7	0
3	E	10	0	10	2	0
3	F	10	0	10	1	0
3	G	10	0	10	2	0
3	H	10	0	8	5	0
3	I	10	0	10	2	0
3	J	10	0	10	2	0
3	K	10	0	10	0	0
3	L	10	0	10	1	0
3	M	10	0	10	2	0
3	N	10	0	10	2	0
3	O	10	0	10	8	0
3	P	10	0	10	6	0
4	A	26	0	0	7	0
4	B	27	0	0	5	0
4	C	30	0	0	3	1
4	D	37	0	0	6	0
4	E	26	0	0	6	0
4	F	36	0	0	8	1
4	G	25	0	0	11	0
4	H	21	0	0	4	0
4	I	20	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	22	0	0	6	0
4	K	21	0	0	2	1
4	L	39	0	0	8	1
4	M	37	0	0	5	0
4	N	29	0	0	6	0
4	O	28	0	0	1	0
4	P	32	0	0	15	0
All	All	27340	0	25734	1464	9

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 29.

All (1464) 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:J:110:GLU:HA	4:J:731:HOH:O	1.31	1.21
1:B:136:CYS:HB3	1:B:200:ILE:O	1.40	1.20
1:I:96:ARG:NH1	4:I:719:HOH:O	1.91	1.02
1:G:116:ASP:HA	4:G:724:HOH:O	1.59	1.02
1:G:243:GLN:HG2	1:K:243:GLN:HB3	1.39	1.01
1:J:77:GLU:OE2	4:J:711:HOH:O	1.79	1.00
1:N:110:GLU:HA	4:N:733:HOH:O	1.61	0.99
1:G:115:SER:CB	1:N:90:ARG:HH22	1.76	0.98
1:G:73:LEU:N	4:G:715:HOH:O	1.94	0.97
1:G:115:SER:HB2	1:N:90:ARG:HH22	1.27	0.97
1:G:243:GLN:HG3	1:K:244:ALA:HB2	1.47	0.95
1:D:83:VAL:HG22	4:D:722:HOH:O	1.66	0.94
1:F:37:ASN:HB3	4:F:728:HOH:O	1.67	0.94
1:A:61:ASN:OD1	4:A:721:HOH:O	1.86	0.92
1:L:98:LEU:O	4:L:750:HOH:O	1.87	0.92
1:C:136:CYS:HB3	1:C:200:ILE:O	1.67	0.92
1:G:110:GLU:OE1	1:N:87:LEU:HG	1.68	0.92
1:P:78:PRO:HG3	4:P:735:HOH:O	1.70	0.91
1:O:77:GLU:OE2	4:O:716:HOH:O	1.88	0.90
1:O:216:GLY:HA3	3:O:715:PBZ:N2	1.86	0.89
1:M:186:GLY:O	4:M:721:HOH:O	1.90	0.89
1:N:217:LYS:NZ	4:N:725:HOH:O	2.04	0.89
1:C:77:GLU:OE2	4:C:715:HOH:O	1.89	0.89
1:B:234:PHE:HA	4:B:703:HOH:O	1.73	0.88
1:C:150:ARG:HD3	1:C:151:MET:H	1.37	0.88
1:G:243:GLN:HG2	1:K:244:ALA:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:27:GLN:OE1	4:L:736:HOH:O	1.93	0.86
1:G:208:TYR:CE2	1:K:125:SER:OG	2.28	0.85
1:E:234:PHE:O	1:E:238:ILE:HG13	1.77	0.84
1:K:177:HIS:HD2	1:K:179:SER:OG	1.61	0.84
1:G:191:CYS:SG	1:G:192:ASN:N	2.50	0.83
1:M:150:ARG:HD3	1:M:151:MET:H	1.43	0.83
1:P:234:PHE:O	1:P:238:ILE:HG13	1.78	0.83
1:F:177:HIS:HD2	1:F:179:SER:OG	1.62	0.82
1:G:186(A):GLN:HG2	1:H:57:HIS:CG	2.14	0.82
1:G:186(A):GLN:HG2	1:H:57:HIS:CD2	2.14	0.82
1:P:78:PRO:CG	4:P:735:HOH:O	2.25	0.82
1:B:201:CYS:HB2	1:B:210:GLN:HE21	1.45	0.82
1:J:150:ARG:HD3	1:J:151:MET:H	1.42	0.82
1:O:150:ARG:HD3	1:O:151:MET:H	1.44	0.82
1:I:187:GLN:HG2	1:I:220(A):GLY:O	1.80	0.81
1:K:136:CYS:HB3	1:K:200:ILE:O	1.81	0.81
1:L:177:HIS:HD2	1:L:179:SER:OG	1.64	0.81
1:M:97:PRO:HB2	4:M:731:HOH:O	1.79	0.80
1:H:177:HIS:HD2	1:H:179:SER:OG	1.64	0.80
1:E:177:HIS:HD2	1:E:179:SER:OG	1.63	0.80
1:O:177:HIS:HD2	1:O:179:SER:OG	1.65	0.80
1:C:166:GLU:OE2	1:E:176:TYR:HE1	1.64	0.80
1:D:37:ASN:O	4:D:716:HOH:O	2.00	0.80
1:D:234:PHE:O	1:D:238:ILE:HG13	1.82	0.80
1:A:136:CYS:HB3	1:A:200:ILE:O	1.82	0.80
1:N:177:HIS:HD2	1:N:179:SER:OG	1.66	0.79
1:A:125:SER:OG	4:A:725:HOH:O	1.99	0.79
1:J:97:PRO:HB2	4:J:724:HOH:O	1.82	0.79
1:G:177:HIS:HD2	1:G:179:SER:OG	1.66	0.79
1:O:234:PHE:O	1:O:238:ILE:HG13	1.81	0.79
1:O:216:GLY:HA3	3:O:715:PBZ:HN22	1.43	0.79
1:M:187:GLN:HG2	1:M:220(A):GLY:O	1.83	0.78
1:I:177:HIS:HD2	1:I:179:SER:OG	1.66	0.78
1:D:187:GLN:HG2	1:D:220(A):GLY:O	1.84	0.78
1:D:190:SER:HB2	3:D:704:PBZ:HN22	1.46	0.78
1:P:177:HIS:HD2	1:P:179:SER:OG	1.66	0.78
1:A:234:PHE:O	1:A:238:ILE:HG13	1.84	0.78
1:C:177:HIS:HD2	1:C:179:SER:OG	1.66	0.78
1:J:187:GLN:HG2	1:J:220(A):GLY:O	1.83	0.78
1:G:115:SER:HB2	1:N:90:ARG:NH2	1.98	0.78
1:C:150:ARG:HD3	1:C:151:MET:N	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:215:PHE:HA	3:P:716:PBZ:C2	2.14	0.78
1:J:177:HIS:HD2	1:J:179:SER:OG	1.64	0.77
1:J:136:CYS:HB3	1:J:200:ILE:O	1.85	0.77
1:P:215:PHE:HA	3:P:716:PBZ:H2	1.67	0.77
1:F:242:VAL:O	4:F:713:HOH:O	2.01	0.76
1:P:78:PRO:CD	4:P:735:HOH:O	2.33	0.76
1:C:93:GLU:HB3	4:C:710:HOH:O	1.84	0.76
1:H:187:GLN:HG2	1:H:220(A):GLY:O	1.85	0.76
1:M:150:ARG:HD3	1:M:151:MET:N	2.00	0.76
1:P:78:PRO:N	4:P:735:HOH:O	2.19	0.76
1:B:57:HIS:NE2	4:B:708:HOH:O	2.19	0.76
1:N:187:GLN:HG2	1:N:220(A):GLY:O	1.85	0.76
1:G:110:GLU:CD	1:N:87:LEU:HG	2.11	0.75
1:J:234:PHE:O	1:J:238:ILE:HG13	1.86	0.75
1:K:166:GLU:OE2	1:M:176:TYR:HE1	1.68	0.75
1:J:150:ARG:HD3	1:J:151:MET:N	2.00	0.75
1:L:234:PHE:O	1:L:238:ILE:HG13	1.86	0.75
1:B:187:GLN:HG2	1:B:220(A):GLY:O	1.85	0.75
1:B:186(A):GLN:HE22	1:C:215:PHE:CB	1.99	0.75
1:H:234:PHE:O	1:H:238:ILE:HG13	1.86	0.75
1:O:187:GLN:HG2	1:O:220(A):GLY:O	1.86	0.75
1:A:177:HIS:HD2	1:A:179:SER:OG	1.69	0.75
1:C:187:GLN:HG2	1:C:220(A):GLY:O	1.85	0.75
1:B:234:PHE:O	1:B:238:ILE:HG13	1.87	0.75
1:G:234:PHE:O	1:G:238:ILE:HG13	1.87	0.75
1:I:234:PHE:O	1:I:238:ILE:HG13	1.87	0.74
1:N:191:CYS:SG	1:N:192:ASN:N	2.60	0.74
1:F:234:PHE:O	1:F:238:ILE:HG13	1.87	0.74
1:J:28:PRO:HB2	1:J:119:ARG:H	1.49	0.74
1:L:187:GLN:HG2	1:L:220(A):GLY:O	1.88	0.74
1:O:150:ARG:HD3	1:O:151:MET:N	2.01	0.74
1:G:28:PRO:HB2	1:G:119:ARG:H	1.52	0.74
1:L:157:CYS:O	1:L:158:VAL:HB	1.88	0.74
1:K:234:PHE:O	1:K:238:ILE:HG13	1.87	0.74
1:F:74:GLU:OE2	4:F:723:HOH:O	2.06	0.73
1:D:177:HIS:HD2	1:D:179:SER:OG	1.72	0.73
1:E:215:PHE:HB3	1:H:186(A):GLN:HE22	1.54	0.73
1:E:215:PHE:CB	1:H:186(A):GLN:HE22	2.02	0.72
1:G:83:VAL:HG21	1:G:108:LEU:HD22	1.70	0.72
1:J:222:VAL:HB	4:J:732:HOH:O	1.88	0.72
1:M:88:SER:OG	4:M:750:HOH:O	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:234:PHE:O	1:N:238:ILE:HG13	1.90	0.72
1:F:187:GLN:HG2	1:F:220(A):GLY:O	1.90	0.72
1:G:115:SER:HA	1:N:90:ARG:NH2	2.05	0.72
1:K:33:LEU:HB2	1:K:42:CYS:O	1.90	0.72
1:A:187:GLN:HG2	1:A:220(A):GLY:O	1.89	0.71
1:E:187:GLN:HG2	1:E:220(A):GLY:O	1.90	0.71
1:M:177:HIS:HD2	1:M:179:SER:OG	1.73	0.71
1:D:120:SER:OG	4:D:715:HOH:O	2.02	0.71
1:F:127:GLN:HA	4:F:725:HOH:O	1.89	0.71
1:P:83:VAL:HG21	1:P:108:LEU:HD22	1.72	0.71
1:I:101:ASN:ND2	4:I:713:HOH:O	2.18	0.71
1:P:187:GLN:HG2	1:P:220(A):GLY:O	1.89	0.71
1:K:187:GLN:HG2	1:K:220(A):GLY:O	1.90	0.71
1:A:28:PRO:HB2	1:A:119:ARG:H	1.54	0.71
1:G:201:CYS:HB3	1:G:210:GLN:HE21	1.56	0.71
1:I:28:PRO:HB2	1:I:119:ARG:H	1.55	0.71
1:L:77:GLU:OE2	4:L:713:HOH:O	2.09	0.71
1:N:201:CYS:HB2	1:N:210:GLN:HE21	1.55	0.71
1:M:234:PHE:O	1:M:238:ILE:HG13	1.90	0.71
1:B:177:HIS:HD2	1:B:179:SER:OG	1.73	0.70
1:K:28:PRO:HB2	1:K:119:ARG:H	1.56	0.70
1:L:28:PRO:HB2	1:L:119:ARG:H	1.57	0.70
1:M:70:LEU:HB2	4:M:735:HOH:O	1.91	0.70
1:N:103:LEU:H	1:N:103:LEU:HD23	1.55	0.70
1:I:186(A):GLN:HE22	1:J:215:PHE:CB	2.04	0.70
1:A:201:CYS:HB2	1:A:210:GLN:HE21	1.56	0.69
1:O:35:MET:O	1:O:36:GLU:C	2.35	0.69
1:O:28:PRO:HB2	1:O:119:ARG:H	1.57	0.69
1:I:186(A):GLN:HE22	1:J:215:PHE:HB3	1.57	0.69
1:M:192:ASN:OD1	3:M:713:PBZ:H2	1.93	0.69
1:N:116:ASP:O	4:N:742:HOH:O	2.11	0.69
1:P:27:GLN:C	4:P:730:HOH:O	2.34	0.69
1:C:234:PHE:O	1:C:238:ILE:HG13	1.92	0.69
1:G:25:HIS:NE2	4:G:716:HOH:O	2.17	0.68
1:E:28:PRO:HB2	1:E:119:ARG:H	1.57	0.68
1:H:28:PRO:HB2	1:H:119:ARG:H	1.59	0.67
1:D:136:CYS:HB3	1:D:200:ILE:O	1.95	0.67
1:D:28:PRO:HB2	1:D:119:ARG:H	1.58	0.67
1:J:50:GLN:HA	1:J:108:LEU:HD12	1.77	0.67
1:E:81:GLN:OE1	4:E:714:HOH:O	2.11	0.67
1:B:28:PRO:HB2	1:B:119:ARG:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:VAL:HG21	1:E:108:LEU:HD22	1.76	0.67
1:K:83:VAL:HG21	1:K:108:LEU:HD22	1.76	0.67
1:B:83:VAL:HG21	1:B:108:LEU:HD22	1.77	0.67
1:D:176:TYR:HE1	1:H:166:GLU:OE2	1.78	0.67
1:D:83:VAL:HG21	1:D:108:LEU:HD22	1.75	0.66
1:F:83:VAL:HG21	1:F:108:LEU:HD22	1.75	0.66
1:P:190:SER:HB2	3:P:716:PBZ:HN32	1.61	0.66
1:P:28:PRO:HB2	1:P:119:ARG:H	1.61	0.66
1:C:28:PRO:HB2	1:C:119:ARG:H	1.60	0.66
1:D:51:TRP:CD1	1:D:242:VAL:HG13	2.30	0.66
1:H:50:GLN:HA	1:H:108:LEU:HD12	1.77	0.66
1:I:83:VAL:HG21	1:I:108:LEU:HD22	1.78	0.66
1:M:28:PRO:HB2	1:M:119:ARG:H	1.61	0.66
1:B:59:PHE:C	1:B:59:PHE:CD2	2.73	0.65
1:A:215:PHE:HA	3:A:701:PBZ:C2	2.26	0.65
1:O:83:VAL:HG21	1:O:108:LEU:HD22	1.78	0.65
1:A:166:GLU:OE2	1:G:176:TYR:HE1	1.80	0.65
1:P:78:PRO:CA	4:P:735:HOH:O	2.44	0.65
1:A:51:TRP:CD1	1:A:242:VAL:HG13	2.32	0.65
1:C:50:GLN:HA	1:C:108:LEU:HD12	1.79	0.65
1:L:59:PHE:C	1:L:59:PHE:CD2	2.75	0.65
1:F:103:LEU:HD23	1:F:103:LEU:H	1.62	0.65
1:J:83:VAL:HG21	1:J:108:LEU:HD22	1.79	0.65
1:D:103:LEU:HD23	1:D:103:LEU:H	1.62	0.65
1:A:83:VAL:HG21	1:A:108:LEU:HD22	1.79	0.65
1:F:116:ASP:HB2	4:F:721:HOH:O	1.97	0.65
1:C:83:VAL:HG21	1:C:108:LEU:HD22	1.77	0.64
1:F:28:PRO:HB2	1:F:119:ARG:H	1.60	0.64
1:F:201:CYS:HB2	1:F:210:GLN:HE21	1.62	0.64
1:N:83:VAL:HG21	1:N:108:LEU:HD22	1.77	0.64
1:G:143:LEU:HD13	1:G:192:ASN:HB2	1.79	0.64
1:F:74:GLU:HG3	4:F:723:HOH:O	1.96	0.64
1:G:243:GLN:HB3	1:K:243:GLN:HG2	1.79	0.64
1:I:177:HIS:ND1	1:I:178:PRO:HD2	2.12	0.64
1:C:143:LEU:HD13	1:C:192:ASN:HB2	1.79	0.64
1:G:35:MET:O	1:G:36:GLU:C	2.41	0.64
1:G:50:GLN:HA	1:G:108:LEU:HD12	1.78	0.64
1:A:35:MET:O	1:A:36:GLU:C	2.41	0.64
1:J:59:PHE:C	1:J:59:PHE:CD2	2.76	0.64
1:D:50:GLN:HA	1:D:108:LEU:HD12	1.80	0.64
1:F:151:MET:HG2	4:F:737:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:MET:O	1:H:36:GLU:C	2.40	0.64
1:I:201:CYS:HB2	1:I:210:GLN:HE21	1.63	0.64
1:P:59:PHE:C	1:P:59:PHE:CD2	2.76	0.64
1:I:59:PHE:C	1:I:59:PHE:CD2	2.76	0.63
1:K:50:GLN:HA	1:K:108:LEU:HD12	1.79	0.63
1:E:85:ALA:HB2	1:E:108:LEU:HA	1.80	0.63
1:G:59:PHE:C	1:G:59:PHE:CD2	2.76	0.63
1:C:35:MET:O	1:C:36:GLU:C	2.40	0.63
1:N:59:PHE:C	1:N:59:PHE:CD2	2.75	0.63
1:J:103:LEU:HD23	1:J:103:LEU:H	1.63	0.63
1:B:50:GLN:HA	1:B:108:LEU:HD12	1.80	0.63
1:E:50:GLN:HA	1:E:108:LEU:HD12	1.80	0.63
1:G:137:LEU:HD11	1:G:157:CYS:HB3	1.79	0.63
1:L:50:GLN:HA	1:L:108:LEU:HD12	1.81	0.63
1:M:83:VAL:HG21	1:M:108:LEU:HD22	1.79	0.63
1:O:50:GLN:HA	1:O:108:LEU:HD12	1.80	0.62
1:B:176:TYR:HE1	1:F:166:GLU:OE2	1.83	0.62
1:D:59:PHE:C	1:D:59:PHE:CD2	2.77	0.62
1:F:74(A):ALA:HB2	1:F:82:MET:HE2	1.81	0.62
1:O:177:HIS:ND1	1:O:178:PRO:HD2	2.14	0.62
1:P:190:SER:C	3:P:716:PBZ:N3	2.57	0.62
1:N:28:PRO:HB2	1:N:119:ARG:H	1.65	0.62
1:P:35:MET:O	1:P:36:GLU:C	2.42	0.62
1:J:190:SER:O	3:J:710:PBZ:N3	2.33	0.62
1:L:83:VAL:HG21	1:L:108:LEU:HD22	1.79	0.62
1:M:59:PHE:C	1:M:59:PHE:CD2	2.77	0.62
1:O:216:GLY:CA	3:O:715:PBZ:HN22	2.13	0.62
1:D:215:PHE:HA	3:D:704:PBZ:C6	2.30	0.62
1:O:59:PHE:C	1:O:59:PHE:CD2	2.77	0.62
1:P:203:GLY:N	4:P:720:HOH:O	2.03	0.62
1:E:51:TRP:CD1	1:E:242:VAL:HG13	2.35	0.62
1:H:85:ALA:HB2	1:H:108:LEU:HA	1.82	0.62
1:L:103:LEU:H	1:L:103:LEU:HD23	1.65	0.62
1:B:40:LEU:HD13	1:B:41:PHE:N	2.15	0.62
1:G:115:SER:CA	1:N:90:ARG:HH22	2.12	0.62
1:A:50:GLN:HA	1:A:108:LEU:HD12	1.82	0.62
1:E:35:MET:O	1:E:36:GLU:C	2.41	0.62
1:H:51:TRP:CD1	1:H:242:VAL:HG13	2.35	0.62
1:B:186(A):GLN:HE22	1:C:215:PHE:HB3	1.64	0.61
1:C:59:PHE:C	1:C:59:PHE:CD2	2.77	0.61
1:K:35:MET:O	1:K:36:GLU:C	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:85:ALA:HB2	1:I:108:LEU:HA	1.82	0.61
1:M:35:MET:O	1:M:36:GLU:C	2.43	0.61
1:F:35:MET:O	1:F:36:GLU:C	2.44	0.61
1:J:231:LEU:C	1:J:233:LYS:H	2.09	0.61
1:P:50:GLN:HA	1:P:108:LEU:HD12	1.81	0.61
1:F:59:PHE:C	1:F:59:PHE:CD2	2.78	0.61
1:N:35:MET:O	1:N:36:GLU:C	2.43	0.61
1:N:143:LEU:HD13	1:N:192:ASN:HB2	1.82	0.61
1:P:103:LEU:HD23	1:P:103:LEU:H	1.64	0.61
1:A:57:HIS:CD2	1:D:186(A):GLN:HG2	2.36	0.61
1:A:103:LEU:HD23	1:A:103:LEU:H	1.66	0.61
1:A:41:PHE:CD2	1:A:42:CYS:SG	2.94	0.61
1:A:41:PHE:HD2	1:A:42:CYS:SG	2.24	0.61
1:C:103:LEU:HD23	1:C:103:LEU:H	1.66	0.61
1:H:136:CYS:HB3	1:H:200:ILE:O	1.99	0.61
1:I:51:TRP:CD1	1:I:242:VAL:HG13	2.36	0.61
1:B:16:ILE:O	4:B:718:HOH:O	2.16	0.61
1:I:50:GLN:HA	1:I:108:LEU:HD12	1.83	0.60
1:J:35:MET:O	1:J:36:GLU:C	2.45	0.60
1:L:177:HIS:ND1	1:L:178:PRO:HD2	2.16	0.60
1:M:177:HIS:ND1	1:M:178:PRO:HD2	2.16	0.60
1:P:51:TRP:CD1	1:P:242:VAL:HG13	2.37	0.60
1:A:220:CYS:SG	3:A:701:PBZ:N2	2.74	0.60
1:B:35:MET:O	1:B:36:GLU:C	2.43	0.60
1:G:79:GLY:O	4:G:714:HOH:O	2.17	0.60
1:H:74(A):ALA:HB2	1:H:82:MET:HE2	1.84	0.60
1:P:146:ASN:ND2	4:P:741:HOH:O	2.33	0.60
1:F:50:GLN:NE2	4:F:720:HOH:O	2.34	0.60
1:M:50:GLN:HA	1:M:108:LEU:HD12	1.84	0.60
1:B:57:HIS:CD2	4:B:708:HOH:O	2.53	0.60
1:D:50:GLN:HG3	1:D:111:SER:HA	1.82	0.60
1:D:35:MET:O	1:D:36:GLU:C	2.44	0.60
1:F:23:SER:O	1:F:26:SER:OG	2.16	0.60
1:K:103:LEU:HD23	1:K:103:LEU:H	1.65	0.60
1:L:90:ARG:NH1	4:L:743:HOH:O	2.34	0.60
1:J:51:TRP:CD1	1:J:242:VAL:HG13	2.37	0.60
1:E:103:LEU:H	1:E:103:LEU:HD23	1.66	0.59
1:G:97:PRO:HB2	4:G:713:HOH:O	2.01	0.59
1:C:191:CYS:O	1:C:192:ASN:C	2.45	0.59
1:M:40:LEU:HD13	1:M:41:PHE:N	2.17	0.59
1:O:51:TRP:CD1	1:O:242:VAL:HG13	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:35:MET:O	1:I:36:GLU:C	2.45	0.59
1:K:59:PHE:CD2	1:K:59:PHE:C	2.79	0.59
1:K:143:LEU:HD13	1:K:192:ASN:HB2	1.83	0.59
1:B:186(A):GLN:HG2	1:C:57:HIS:CD2	2.37	0.59
1:C:142:GLY:N	1:C:194:ASP:OD1	2.35	0.59
1:G:51:TRP:CD1	1:G:242:VAL:HG13	2.38	0.59
1:G:59:PHE:HB2	1:G:90:ARG:HD3	1.85	0.59
1:L:35:MET:O	1:L:36:GLU:C	2.43	0.59
1:L:51:TRP:CD1	1:L:242:VAL:HG13	2.37	0.59
1:C:74(A):ALA:HB2	1:C:82:MET:HE2	1.85	0.59
1:M:85:ALA:HB2	1:M:108:LEU:HA	1.85	0.59
1:O:192:ASN:OD1	3:O:715:PBZ:H2	2.02	0.59
1:P:74(A):ALA:HB2	1:P:82:MET:HE2	1.85	0.59
1:B:50:GLN:HG3	1:B:111:SER:HA	1.85	0.59
1:D:74(A):ALA:HB2	1:D:82:MET:HE2	1.83	0.59
1:F:50:GLN:HA	1:F:108:LEU:HD12	1.84	0.59
1:K:177:HIS:HB3	1:K:180:MET:HE3	1.83	0.59
1:B:40:LEU:HD13	1:B:40:LEU:C	2.27	0.59
1:D:85:ALA:HB2	1:D:108:LEU:HA	1.83	0.59
1:D:151:MET:HG2	4:D:728:HOH:O	2.02	0.59
1:K:85:ALA:HB2	1:K:108:LEU:HA	1.85	0.59
1:L:143:LEU:HD13	1:L:192:ASN:HB2	1.84	0.59
1:P:177:HIS:ND1	1:P:178:PRO:HD2	2.18	0.59
1:B:218:ALA:HA	1:B:219:PRO:C	2.28	0.58
1:H:25:HIS:NE2	4:H:717:HOH:O	2.21	0.58
1:M:143:LEU:HD13	1:M:192:ASN:HB2	1.83	0.58
1:P:85:ALA:HB2	1:P:108:LEU:HA	1.85	0.58
1:K:50:GLN:HG3	1:K:111:SER:HA	1.85	0.58
1:L:74(A):ALA:HB2	1:L:82:MET:HE2	1.83	0.58
1:D:190:SER:C	3:D:704:PBZ:N2	2.61	0.58
1:N:74(A):ALA:HB2	1:N:82:MET:HE2	1.84	0.58
1:F:85:ALA:HB2	1:F:108:LEU:HA	1.85	0.58
1:J:74(A):ALA:HB2	1:J:82:MET:HE2	1.85	0.58
1:L:180:MET:HB3	4:L:746:HOH:O	2.02	0.58
1:C:50:GLN:HG3	1:C:111:SER:HA	1.85	0.58
1:G:243:GLN:HG3	1:K:244:ALA:CB	2.28	0.58
1:H:191:CYS:HA	3:H:708:PBZ:HN32	1.68	0.58
1:A:85:ALA:HB2	1:A:108:LEU:HA	1.84	0.58
1:D:177:HIS:ND1	1:D:178:PRO:HD2	2.18	0.58
1:H:177:HIS:HB3	1:H:180:MET:HE3	1.84	0.58
1:I:59:PHE:HB2	1:I:90:ARG:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ASN:ND2	1:K:116:ASP:OD2	2.36	0.58
1:K:51:TRP:CD1	1:K:242:VAL:HG13	2.39	0.58
1:O:98:LEU:O	1:O:99:LEU:HB2	2.04	0.58
1:C:40:LEU:C	1:C:40:LEU:HD13	2.29	0.58
1:D:98:LEU:HG	1:D:99:LEU:HG	1.86	0.58
1:G:115:SER:CB	1:N:90:ARG:NH2	2.58	0.58
1:K:177:HIS:ND1	1:K:178:PRO:HD2	2.19	0.58
1:P:78:PRO:O	1:P:80:SER:N	2.36	0.58
1:A:177:HIS:ND1	1:A:178:PRO:HD2	2.18	0.58
1:J:231:LEU:C	1:J:233:LYS:N	2.60	0.58
1:M:40:LEU:HD13	1:M:40:LEU:C	2.29	0.58
1:M:51:TRP:CD1	1:M:242:VAL:HG13	2.39	0.58
1:G:74(A):ALA:HB2	1:G:82:MET:HE2	1.84	0.57
1:G:177:HIS:ND1	1:G:178:PRO:HD2	2.19	0.57
1:B:103:LEU:H	1:B:103:LEU:HD23	1.68	0.57
1:E:177:HIS:HB3	1:E:180:MET:HE3	1.85	0.57
1:N:59:PHE:HB2	1:N:90:ARG:HD3	1.85	0.57
1:B:51:TRP:CD1	1:B:242:VAL:HG13	2.39	0.57
1:C:218:ALA:HA	1:C:219:PRO:C	2.30	0.57
1:E:177:HIS:ND1	1:E:178:PRO:HD2	2.19	0.57
1:H:59:PHE:C	1:H:59:PHE:CD2	2.81	0.57
1:N:50:GLN:HA	1:N:108:LEU:HD12	1.84	0.57
1:D:59:PHE:HB2	1:D:90:ARG:HD3	1.86	0.57
1:E:59:PHE:C	1:E:59:PHE:CD2	2.82	0.57
1:I:40:LEU:HD13	1:I:41:PHE:N	2.20	0.57
1:I:74(A):ALA:HB2	1:I:82:MET:HE2	1.84	0.57
1:N:40:LEU:HD13	1:N:40:LEU:C	2.29	0.57
1:G:85:ALA:HB2	1:G:108:LEU:HA	1.85	0.57
1:C:51:TRP:CZ3	1:C:107:LYS:HB2	2.40	0.57
1:F:143:LEU:HD13	1:F:192:ASN:HB2	1.86	0.57
1:G:218:ALA:HA	1:G:219:PRO:C	2.29	0.57
1:J:177:HIS:ND1	1:J:178:PRO:HD2	2.19	0.57
1:K:98:LEU:O	1:K:99:LEU:HB2	2.03	0.57
1:N:85:ALA:HB2	1:N:108:LEU:HA	1.86	0.57
1:A:218:ALA:HA	1:A:219:PRO:C	2.28	0.57
1:C:85:ALA:HB2	1:C:108:LEU:HA	1.86	0.57
1:C:177:HIS:ND1	1:C:178:PRO:HD2	2.19	0.57
1:F:51:TRP:CD1	1:F:242:VAL:HG13	2.40	0.57
1:D:40:LEU:HD13	1:D:41:PHE:N	2.20	0.57
1:F:78:PRO:O	1:F:80:SER:N	2.38	0.57
1:I:220:CYS:SG	3:I:709:PBZ:H5	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:59:PHE:HB2	1:O:90:ARG:HD3	1.87	0.57
1:E:218:ALA:HA	1:E:219:PRO:C	2.29	0.57
1:H:177:HIS:ND1	1:H:178:PRO:HD2	2.19	0.57
1:N:40:LEU:HD13	1:N:41:PHE:N	2.20	0.57
1:P:190:SER:O	3:P:716:PBZ:N3	2.38	0.57
1:I:177:HIS:HE1	4:I:728:HOH:O	1.87	0.56
1:A:98:LEU:O	1:A:99:LEU:HB2	2.05	0.56
1:D:51:TRP:CZ3	1:D:107:LYS:HB2	2.39	0.56
1:D:201:CYS:HB2	1:D:210:GLN:HE21	1.69	0.56
1:E:59:PHE:HB2	1:E:90:ARG:HD3	1.87	0.56
1:G:27:GLN:N	4:G:719:HOH:O	2.18	0.56
1:I:218:ALA:HA	1:I:219:PRO:C	2.29	0.56
1:J:191:CYS:HA	3:J:710:PBZ:HN32	1.70	0.56
1:K:186(A):GLN:HG2	1:L:57:HIS:CD2	2.41	0.56
1:L:136:CYS:HB3	1:L:200:ILE:O	2.05	0.56
1:O:85:ALA:HB2	1:O:108:LEU:HA	1.87	0.56
1:P:48:HIS:CG	1:P:49:PRO:HD2	2.40	0.56
1:B:59:PHE:HB2	1:B:90:ARG:HD3	1.88	0.56
1:E:112:VAL:HG12	4:E:714:HOH:O	2.05	0.56
1:G:40:LEU:HD13	1:G:40:LEU:C	2.31	0.56
1:J:59:PHE:HB2	1:J:90:ARG:HD3	1.87	0.56
1:C:51:TRP:CD1	1:C:242:VAL:HG13	2.40	0.56
1:E:51:TRP:CZ3	1:E:107:LYS:HB2	2.40	0.56
1:I:128:CYS:HB3	1:I:129:PRO:CD	2.35	0.56
1:J:85:ALA:HB2	1:J:108:LEU:HA	1.88	0.56
1:C:40:LEU:HD13	1:C:41:PHE:N	2.21	0.56
1:G:127:GLN:HB2	1:K:208:TYR:OH	2.06	0.56
1:L:35:MET:HG2	1:L:41:PHE:CE1	2.40	0.56
1:E:136:CYS:HB3	1:E:200:ILE:O	2.06	0.56
1:F:40:LEU:HD13	1:F:40:LEU:C	2.31	0.56
1:J:187:GLN:HA	4:J:729:HOH:O	2.06	0.56
1:J:191:CYS:O	1:J:192:ASN:C	2.49	0.56
1:J:218:ALA:HA	1:J:219:PRO:C	2.30	0.56
1:A:48:HIS:CG	1:A:49:PRO:HD2	2.41	0.56
1:B:74(A):ALA:HB2	1:B:82:MET:HE2	1.87	0.56
1:F:215:PHE:HA	3:F:706:PBZ:C6	2.36	0.56
1:H:103:LEU:HD23	1:H:103:LEU:H	1.70	0.56
1:K:231:LEU:C	1:K:233:LYS:H	2.14	0.56
1:A:49:PRO:O	1:A:112:VAL:HG22	2.06	0.56
1:A:50:GLN:HG3	1:A:111:SER:HA	1.86	0.56
1:A:74(A):ALA:HB2	1:A:82:MET:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:SER:O	1:D:26:SER:OG	2.22	0.56
1:J:48:HIS:CG	1:J:49:PRO:HD2	2.41	0.56
1:N:48:HIS:CG	1:N:49:PRO:HD2	2.41	0.56
1:O:136:CYS:HB3	1:O:200:ILE:O	2.05	0.56
1:A:128:CYS:O	1:A:129:PRO:C	2.47	0.55
1:E:182:CYS:HB3	1:E:225:PRO:HB2	1.88	0.55
1:G:243:GLN:CG	1:K:244:ALA:H	2.16	0.55
1:K:59:PHE:HB2	1:K:90:ARG:HD3	1.88	0.55
1:L:59:PHE:HB2	1:L:90:ARG:HD3	1.87	0.55
1:L:235:THR:HG22	4:L:722:HOH:O	2.06	0.55
1:N:51:TRP:CD1	1:N:242:VAL:HG13	2.41	0.55
1:F:48:HIS:CG	1:F:49:PRO:HD2	2.41	0.55
1:L:85:ALA:HB2	1:L:108:LEU:HA	1.88	0.55
1:L:122:SER:HB3	4:L:730:HOH:O	2.06	0.55
1:A:142:GLY:N	1:A:194:ASP:OD1	2.38	0.55
1:P:50:GLN:HG3	1:P:111:SER:HA	1.89	0.55
1:N:23:SER:O	1:N:26:SER:OG	2.21	0.55
1:E:48:HIS:CG	1:E:49:PRO:HD2	2.40	0.55
1:G:115:SER:CA	1:N:90:ARG:NH2	2.68	0.55
1:J:40:LEU:HD13	1:J:41:PHE:N	2.21	0.55
1:J:142:GLY:N	1:J:194:ASP:OD1	2.39	0.55
1:O:192:ASN:HA	3:O:715:PBZ:HN11	1.72	0.55
1:O:220:CYS:SG	3:O:715:PBZ:H3	2.47	0.55
1:C:78:PRO:O	1:C:80:SER:N	2.40	0.55
1:F:177:HIS:HB3	1:F:180:MET:HE3	1.89	0.55
1:N:50:GLN:HG3	1:N:111:SER:HA	1.89	0.55
1:N:177:HIS:ND1	1:N:178:PRO:HD2	2.22	0.55
1:O:74(A):ALA:HB2	1:O:82:MET:HE2	1.88	0.55
1:B:48:HIS:CG	1:B:49:PRO:HD2	2.41	0.55
1:J:40:LEU:HD13	1:J:40:LEU:C	2.32	0.55
1:E:98:LEU:HG	1:E:99:LEU:HG	1.89	0.55
1:F:50:GLN:HG3	1:F:111:SER:HA	1.88	0.55
1:G:40:LEU:HD13	1:G:41:PHE:N	2.21	0.55
1:I:97:PRO:HB2	4:I:725:HOH:O	2.06	0.55
1:O:51:TRP:CZ3	1:O:107:LYS:HB2	2.42	0.55
1:A:78:PRO:O	1:A:80:SER:N	2.40	0.55
1:M:78:PRO:O	1:M:80:SER:N	2.40	0.55
1:B:51:TRP:CZ3	1:B:107:LYS:HB2	2.42	0.55
1:G:35:MET:HG2	1:G:41:PHE:CE1	2.42	0.55
1:H:35:MET:HG2	1:H:41:PHE:CE1	2.42	0.55
1:H:51:TRP:CZ3	1:H:107:LYS:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:48:HIS:ND1	1:J:49:PRO:HD2	2.22	0.55
1:L:142:GLY:N	1:L:194:ASP:OD1	2.40	0.55
1:B:48:HIS:ND1	1:B:49:PRO:HD2	2.21	0.54
1:I:40:LEU:HD13	1:I:40:LEU:C	2.32	0.54
1:G:48:HIS:ND1	1:G:49:PRO:HD2	2.23	0.54
1:G:243:GLN:CB	1:K:243:GLN:HG2	2.36	0.54
1:J:50:GLN:HG3	1:J:111:SER:HA	1.88	0.54
1:P:177:HIS:HB3	1:P:180:MET:HE3	1.87	0.54
1:F:78:PRO:C	1:F:80:SER:H	2.16	0.54
1:G:78:PRO:O	1:G:80:SER:N	2.40	0.54
1:J:28:PRO:HB2	1:J:119:ARG:N	2.20	0.54
1:M:74(A):ALA:HB2	1:M:82:MET:HE2	1.89	0.54
1:O:177:HIS:HB3	1:O:180:MET:HE3	1.90	0.54
1:A:78:PRO:C	1:A:80:SER:H	2.15	0.54
1:G:50:GLN:HG3	1:G:111:SER:HA	1.89	0.54
1:I:192:ASN:OD1	3:I:709:PBZ:H6	2.06	0.54
1:C:59:PHE:HB2	1:C:90:ARG:HD3	1.88	0.54
1:K:51:TRP:CZ3	1:K:107:LYS:HB2	2.41	0.54
1:K:218:ALA:HA	1:K:219:PRO:C	2.33	0.54
1:P:45:VAL:HG11	1:P:209:LEU:HD22	1.89	0.54
1:A:51:TRP:CZ3	1:A:107:LYS:HB2	2.42	0.54
1:N:218:ALA:HA	1:N:219:PRO:C	2.33	0.54
1:E:35:MET:HG2	1:E:41:PHE:CE1	2.42	0.54
1:E:78:PRO:O	1:E:80:SER:N	2.41	0.54
1:G:110:GLU:OE1	1:N:87:LEU:CG	2.51	0.54
1:P:125:SER:OG	4:P:724:HOH:O	1.96	0.54
1:C:35:MET:HG2	1:C:41:PHE:CE1	2.43	0.54
1:F:48:HIS:ND1	1:F:49:PRO:HD2	2.22	0.54
1:I:50:GLN:HG3	1:I:111:SER:HA	1.89	0.54
1:K:40:LEU:HD13	1:K:40:LEU:C	2.33	0.54
1:K:40:LEU:HD13	1:K:41:PHE:N	2.23	0.54
1:M:166:GLU:O	1:M:167:VAL:C	2.48	0.54
1:O:35:MET:HG2	1:O:41:PHE:CE1	2.43	0.54
1:D:231:LEU:C	1:D:233:LYS:H	2.15	0.54
1:I:51:TRP:CZ3	1:I:107:LYS:HB2	2.43	0.54
1:O:50:GLN:HG3	1:O:111:SER:HA	1.90	0.54
1:E:48:HIS:HB3	1:E:51:TRP:HB2	1.90	0.54
1:F:98:LEU:HG	1:F:99:LEU:HG	1.89	0.54
1:N:98:LEU:HG	1:N:99:LEU:HG	1.90	0.54
1:A:28:PRO:HB2	1:A:119:ARG:N	2.23	0.53
1:D:48:HIS:CG	1:D:49:PRO:HD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:SER:CB	4:E:715:HOH:O	2.57	0.53
1:F:218:ALA:HA	1:F:219:PRO:C	2.32	0.53
1:G:136:CYS:O	1:G:159:ASN:HA	2.07	0.53
1:H:40:LEU:C	1:H:40:LEU:HD13	2.33	0.53
1:L:40:LEU:HD13	1:L:40:LEU:C	2.33	0.53
1:P:78:PRO:C	1:P:80:SER:H	2.14	0.53
1:F:177:HIS:ND1	1:F:178:PRO:HD2	2.23	0.53
1:L:40:LEU:HD13	1:L:41:PHE:N	2.24	0.53
1:M:48:HIS:CG	1:M:49:PRO:HD2	2.43	0.53
1:P:142:GLY:N	1:P:194:ASP:OD1	2.40	0.53
1:F:40:LEU:HD13	1:F:41:PHE:N	2.23	0.53
1:G:23:SER:O	1:G:26:SER:OG	2.25	0.53
1:L:182:CYS:HA	1:L:226:GLY:O	2.09	0.53
1:F:128:CYS:HB3	1:F:129:PRO:CD	2.38	0.53
1:G:27:GLN:C	4:G:719:HOH:O	2.51	0.53
1:M:50:GLN:HG3	1:M:111:SER:HA	1.89	0.53
1:O:98:LEU:HG	1:O:99:LEU:HG	1.90	0.53
1:P:51:TRP:CZ3	1:P:107:LYS:HB2	2.44	0.53
1:P:59:PHE:HB2	1:P:90:ARG:HD3	1.90	0.53
1:D:40:LEU:HD13	1:D:40:LEU:C	2.34	0.53
1:F:59:PHE:HB2	1:F:90:ARG:HD3	1.89	0.53
1:M:38:GLU:HG2	1:M:40:LEU:N	2.24	0.53
1:C:182:CYS:HB3	1:C:225:PRO:HB2	1.90	0.53
1:E:40:LEU:C	1:E:40:LEU:HD13	2.34	0.53
1:G:200:ILE:HA	1:G:208:TYR:O	2.08	0.53
1:I:28:PRO:HB2	1:I:119:ARG:N	2.23	0.53
1:J:186(A):GLN:HG2	1:K:57:HIS:CD2	2.44	0.53
1:M:35:MET:HG2	1:M:41:PHE:CE1	2.44	0.53
1:O:201:CYS:HB2	1:O:210:GLN:HE21	1.74	0.53
1:E:142:GLY:N	1:E:194:ASP:OD1	2.39	0.53
1:F:87:LEU:C	1:F:87:LEU:HD23	2.33	0.53
1:L:218:ALA:HA	1:L:219:PRO:C	2.33	0.53
1:B:166:GLU:OE2	1:F:176:TYR:HE1	1.91	0.53
1:I:38:GLU:HG2	1:I:40:LEU:N	2.24	0.53
1:K:23:SER:O	1:K:26:SER:OG	2.26	0.53
1:L:23:SER:O	1:L:24:PRO:C	2.52	0.53
1:C:48:HIS:ND1	1:C:49:PRO:HD2	2.25	0.52
1:I:103:LEU:HD23	1:I:103:LEU:H	1.73	0.52
1:O:218:ALA:HA	1:O:219:PRO:C	2.34	0.52
1:D:25:HIS:NE2	4:D:724:HOH:O	2.13	0.52
1:G:48:HIS:CG	1:G:49:PRO:HD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:PHE:HA	4:G:717:HOH:O	2.08	0.52
1:M:48:HIS:ND1	1:M:49:PRO:HD2	2.24	0.52
1:B:142:GLY:N	1:B:194:ASP:OD1	2.40	0.52
1:L:50:GLN:HG3	1:L:111:SER:HA	1.89	0.52
1:P:197:GLY:O	1:P:212:LEU:HA	2.09	0.52
1:I:78:PRO:O	1:I:80:SER:N	2.43	0.52
1:B:85:ALA:HB2	1:B:108:LEU:HA	1.91	0.52
1:G:142:GLY:N	1:G:194:ASP:OD1	2.41	0.52
1:G:243:GLN:HB3	1:K:243:GLN:CG	2.39	0.52
1:J:35:MET:HG2	1:J:41:PHE:CE1	2.45	0.52
1:C:98:LEU:O	1:C:99:LEU:HB2	2.10	0.52
1:K:25:HIS:NE2	4:K:719:HOH:O	2.26	0.52
1:K:98:LEU:HG	1:K:99:LEU:HG	1.92	0.52
1:M:59:PHE:HB2	1:M:90:ARG:HD3	1.89	0.52
1:K:48:HIS:CG	1:K:49:PRO:HD2	2.45	0.52
1:N:87:LEU:C	1:N:87:LEU:CD2	2.83	0.52
1:O:186(A):GLN:HG2	1:P:57:HIS:CG	2.45	0.52
1:E:40:LEU:HD13	1:E:41:PHE:N	2.24	0.52
1:L:48:HIS:CG	1:L:49:PRO:HD2	2.44	0.52
1:L:231:LEU:C	1:L:233:LYS:H	2.18	0.52
1:A:98:LEU:HG	1:A:99:LEU:HG	1.91	0.52
1:B:78:PRO:O	1:B:80:SER:N	2.43	0.52
1:B:197:GLY:O	1:B:212:LEU:HA	2.10	0.52
1:C:186(A):GLN:HG2	1:D:57:HIS:CD2	2.45	0.52
1:C:197:GLY:O	1:C:212:LEU:HA	2.10	0.52
1:G:51:TRP:CZ3	1:G:107:LYS:HB2	2.45	0.52
1:I:48:HIS:HB3	1:I:51:TRP:HB2	1.92	0.52
1:O:23:SER:O	1:O:24:PRO:C	2.53	0.52
1:P:27:GLN:N	4:P:730:HOH:O	2.34	0.52
1:C:78:PRO:C	1:C:80:SER:H	2.18	0.52
1:D:78:PRO:O	1:D:80:SER:N	2.43	0.52
1:E:45:VAL:HG11	1:E:209:LEU:HD22	1.91	0.52
1:E:115:SER:HB3	4:E:726:HOH:O	2.10	0.52
1:G:197:GLY:O	1:G:212:LEU:HA	2.09	0.52
1:K:78:PRO:O	1:K:80:SER:N	2.43	0.52
1:N:78:PRO:O	1:N:80:SER:N	2.43	0.52
1:B:177:HIS:ND1	1:B:178:PRO:HD2	2.24	0.51
1:H:40:LEU:HD13	1:H:41:PHE:N	2.24	0.51
1:A:61:ASN:HA	4:A:721:HOH:O	2.11	0.51
1:I:197:GLY:O	1:I:212:LEU:HA	2.10	0.51
1:M:55:ALA:O	1:M:58:CYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ALA:HA	1:D:219:PRO:C	2.35	0.51
1:F:123:ILE:HG12	1:F:209:LEU:HD23	1.93	0.51
1:F:186(A):GLN:HG2	1:G:57:HIS:CD2	2.46	0.51
1:L:48:HIS:HB3	1:L:51:TRP:HB2	1.91	0.51
1:L:51:TRP:CZ3	1:L:107:LYS:HB2	2.45	0.51
1:O:40:LEU:C	1:O:40:LEU:HD13	2.36	0.51
1:A:231:LEU:C	1:A:233:LYS:N	2.64	0.51
1:B:98:LEU:O	1:B:99:LEU:HB2	2.10	0.51
1:G:103:LEU:H	1:G:103:LEU:HD23	1.74	0.51
1:J:51:TRP:CZ3	1:J:107:LYS:HB2	2.45	0.51
1:K:28:PRO:HB2	1:K:119:ARG:N	2.23	0.51
1:K:41:PHE:CE2	1:K:42:CYS:HB2	2.46	0.51
1:P:136:CYS:HB3	1:P:200:ILE:O	2.10	0.51
1:A:112:VAL:HA	4:A:710:HOH:O	2.11	0.51
1:G:28:PRO:HB2	1:G:119:ARG:N	2.21	0.51
1:J:23:SER:O	1:J:26:SER:OG	2.25	0.51
1:M:218:ALA:HA	1:M:219:PRO:C	2.35	0.51
1:N:98:LEU:O	1:N:99:LEU:HB2	2.09	0.51
1:P:40:LEU:HD13	1:P:40:LEU:C	2.36	0.51
1:C:146:ASN:OD1	1:C:150:ARG:HB2	2.10	0.51
1:F:197:GLY:O	1:F:212:LEU:HA	2.10	0.51
1:H:78:PRO:O	1:H:80:SER:N	2.44	0.51
1:I:91:HIS:CG	1:I:92:PRO:HD2	2.46	0.51
1:J:78:PRO:O	1:J:80:SER:N	2.43	0.51
1:N:197:GLY:O	1:N:212:LEU:HA	2.10	0.51
1:O:40:LEU:HD13	1:O:41:PHE:N	2.25	0.51
1:B:78:PRO:C	1:B:80:SER:H	2.19	0.51
1:D:98:LEU:O	1:D:99:LEU:HB2	2.09	0.51
1:H:197:GLY:O	1:H:212:LEU:HA	2.10	0.51
1:N:48:HIS:ND1	1:N:49:PRO:HD2	2.26	0.51
1:P:218:ALA:HA	1:P:219:PRO:C	2.35	0.51
1:B:48:HIS:CE1	1:B:49:PRO:HD2	2.46	0.51
1:C:48:HIS:CG	1:C:49:PRO:HD2	2.45	0.51
1:C:166:GLU:OE2	1:E:176:TYR:CE1	2.55	0.51
1:D:78:PRO:C	1:D:80:SER:H	2.19	0.51
1:D:91:HIS:CG	1:D:92:PRO:HD2	2.46	0.51
1:E:62:SER:HB2	4:E:715:HOH:O	2.10	0.51
1:H:37:ASN:HB2	4:H:726:HOH:O	2.09	0.51
1:H:231:LEU:C	1:H:233:LYS:H	2.19	0.51
1:I:78:PRO:C	1:I:80:SER:H	2.19	0.51
1:K:48:HIS:HB3	1:K:51:TRP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:98:LEU:HG	1:L:99:LEU:HG	1.92	0.51
1:O:186(A):GLN:HG2	1:P:57:HIS:CD2	2.46	0.51
1:C:28:PRO:HB2	1:C:119:ARG:N	2.26	0.51
1:I:48:HIS:CG	1:I:49:PRO:HD2	2.45	0.51
1:K:78:PRO:C	1:K:80:SER:H	2.18	0.51
1:L:177:HIS:HB3	1:L:180:MET:HE3	1.93	0.51
1:G:201:CYS:CB	1:G:210:GLN:HE21	2.24	0.51
1:K:74(A):ALA:HB2	1:K:82:MET:HE2	1.93	0.51
1:E:74(A):ALA:HB2	1:E:82:MET:HE2	1.93	0.50
1:H:216:GLY:HA3	3:H:708:PBZ:N2	2.26	0.50
1:L:45:VAL:HG11	1:L:209:LEU:HD22	1.94	0.50
1:N:78:PRO:C	1:N:80:SER:H	2.19	0.50
1:I:177:HIS:HB3	1:I:180:MET:HE3	1.93	0.50
1:J:98:LEU:O	1:J:99:LEU:HB2	2.11	0.50
1:K:23:SER:O	1:K:24:PRO:C	2.54	0.50
1:N:87:LEU:C	1:N:87:LEU:HD23	2.36	0.50
1:N:103:LEU:HD23	1:N:103:LEU:N	2.23	0.50
1:A:48:HIS:HB3	1:A:51:TRP:HB2	1.93	0.50
1:G:87:LEU:C	1:G:87:LEU:HD23	2.36	0.50
1:J:78:PRO:C	1:J:80:SER:H	2.20	0.50
1:J:197:GLY:O	1:J:212:LEU:HA	2.11	0.50
1:L:48:HIS:ND1	1:L:49:PRO:HD2	2.27	0.50
1:M:78:PRO:C	1:M:80:SER:H	2.19	0.50
1:N:191:CYS:CB	1:N:220:CYS:HG	2.25	0.50
1:P:49:PRO:O	1:P:112:VAL:HG22	2.12	0.50
1:A:59:PHE:O	1:A:60:GLN:NE2	2.44	0.50
1:F:87:LEU:C	1:F:87:LEU:CD2	2.84	0.50
1:G:78:PRO:C	1:G:80:SER:H	2.19	0.50
1:G:177:HIS:HB3	1:G:180:MET:HE3	1.93	0.50
1:J:98:LEU:HG	1:J:99:LEU:HG	1.93	0.50
1:M:51:TRP:CZ3	1:M:107:LYS:HB2	2.46	0.50
1:N:189:ASP:HB2	4:N:717:HOH:O	2.11	0.50
1:O:48:HIS:CG	1:O:49:PRO:HD2	2.46	0.50
1:P:40:LEU:HD13	1:P:41:PHE:N	2.25	0.50
1:A:91:HIS:CG	1:A:92:PRO:HD2	2.46	0.50
1:B:98:LEU:HG	1:B:99:LEU:HG	1.92	0.50
1:C:98:LEU:HG	1:C:99:LEU:HG	1.93	0.50
1:L:231:LEU:C	1:L:233:LYS:N	2.68	0.50
1:P:35:MET:HG2	1:P:41:PHE:CE1	2.47	0.50
1:P:48:HIS:ND1	1:P:49:PRO:HD2	2.26	0.50
1:D:231:LEU:C	1:D:233:LYS:N	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:PRO:C	1:E:80:SER:H	2.19	0.50
1:F:49:PRO:O	1:F:112:VAL:HG22	2.12	0.50
1:H:142:GLY:N	1:H:194:ASP:OD1	2.41	0.50
1:N:191:CYS:HA	1:N:220:CYS:SG	2.52	0.50
1:P:191:CYS:SG	1:P:192:ASN:N	2.85	0.50
1:D:35:MET:HG2	1:D:41:PHE:CE1	2.47	0.50
1:H:49:PRO:O	1:H:112:VAL:HG22	2.11	0.50
1:K:38:GLU:HG2	1:K:40:LEU:N	2.27	0.50
1:L:200:ILE:HA	1:L:208:TYR:O	2.12	0.50
1:A:170:LYS:HB2	1:B:174:PRO:HG3	1.94	0.50
1:B:215:PHE:HA	3:B:702:PBZ:C1	2.42	0.50
1:E:182:CYS:HA	1:E:226:GLY:O	2.12	0.50
1:H:91:HIS:O	1:H:92:PRO:C	2.55	0.50
1:G:87:LEU:C	1:G:87:LEU:CD2	2.85	0.50
1:J:123:ILE:HG12	1:J:209:LEU:HD23	1.94	0.50
1:M:98:LEU:HG	1:M:99:LEU:HG	1.93	0.50
1:N:51:TRP:CZ3	1:N:107:LYS:HB2	2.46	0.50
1:O:49:PRO:O	1:O:112:VAL:HG22	2.11	0.50
1:C:45:VAL:HG11	1:C:209:LEU:HD22	1.93	0.49
1:F:98:LEU:O	1:F:99:LEU:HB2	2.13	0.49
1:H:78:PRO:C	1:H:80:SER:H	2.19	0.49
1:H:98:LEU:HG	1:H:99:LEU:HG	1.93	0.49
1:J:95:ASN:C	1:J:96:ARG:HG2	2.37	0.49
1:M:231:LEU:O	1:M:232:CYS:C	2.49	0.49
1:N:35:MET:HG2	1:N:41:PHE:CE1	2.47	0.49
1:C:49:PRO:O	1:C:112:VAL:HG22	2.12	0.49
1:C:87:LEU:C	1:C:87:LEU:HD23	2.37	0.49
1:C:177:HIS:HB3	1:C:180:MET:HE3	1.94	0.49
1:E:59:PHE:O	1:E:60:GLN:NE2	2.44	0.49
1:E:137:LEU:HD11	1:E:157:CYS:HB3	1.93	0.49
1:F:35:MET:HG2	1:F:41:PHE:CE1	2.47	0.49
1:H:48:HIS:CG	1:H:49:PRO:HD2	2.46	0.49
1:K:128:CYS:HB3	1:K:129:PRO:CD	2.42	0.49
1:M:87:LEU:C	1:M:87:LEU:HD23	2.37	0.49
1:A:23:SER:O	1:A:26:SER:OG	2.29	0.49
1:A:48:HIS:ND1	1:A:49:PRO:HD2	2.26	0.49
1:C:165:GLU:HB3	1:E:165:GLU:HB3	1.94	0.49
1:G:49:PRO:O	1:G:112:VAL:HG22	2.11	0.49
1:K:45:VAL:HG11	1:K:209:LEU:HD22	1.93	0.49
1:K:91:HIS:CG	1:K:92:PRO:HD2	2.46	0.49
1:A:48:HIS:NE2	4:A:723:HOH:O	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:CYS:HB2	1:H:210:GLN:HE21	1.77	0.49
1:K:142:GLY:N	1:K:194:ASP:OD1	2.42	0.49
1:N:17:ILE:HG13	1:N:220:CYS:HB3	1.94	0.49
1:N:123:ILE:HG12	1:N:209:LEU:HD23	1.93	0.49
1:N:215:PHE:HA	3:N:714:PBZ:C6	2.43	0.49
1:F:51:TRP:CZ3	1:F:107:LYS:HB2	2.47	0.49
1:I:59:PHE:O	1:I:60:GLN:NE2	2.46	0.49
1:I:128:CYS:HB3	1:I:129:PRO:HD2	1.93	0.49
1:K:35:MET:HG2	1:K:41:PHE:CE1	2.48	0.49
1:K:231:LEU:C	1:K:233:LYS:N	2.71	0.49
1:L:78:PRO:C	1:L:80:SER:H	2.21	0.49
1:O:170:LYS:HB2	1:P:174:PRO:HG3	1.94	0.49
1:P:98:LEU:O	1:P:99:LEU:HB2	2.12	0.49
1:C:56:ALA:C	1:C:58:CYS:H	2.21	0.49
1:C:61:ASN:O	4:C:728:HOH:O	2.19	0.49
1:L:28:PRO:HB2	1:L:119:ARG:N	2.25	0.49
1:D:45:VAL:HG11	1:D:209:LEU:HD22	1.95	0.49
1:F:128:CYS:HB3	1:F:129:PRO:HD2	1.95	0.49
1:H:123:ILE:HG12	1:H:209:LEU:HD23	1.95	0.49
1:J:87:LEU:HD23	1:J:87:LEU:C	2.38	0.49
1:L:78:PRO:O	1:L:80:SER:N	2.46	0.49
1:A:165:GLU:HB3	1:G:165:GLU:HB3	1.94	0.49
1:B:48:HIS:CG	1:B:49:PRO:CD	2.96	0.49
1:B:87:LEU:C	1:B:87:LEU:HD23	2.37	0.49
1:D:142:GLY:N	1:D:194:ASP:OD1	2.42	0.49
1:G:190:SER:O	3:G:707:PBZ:N3	2.46	0.49
1:H:93:GLU:O	1:H:94:TYR:C	2.53	0.49
1:J:38:GLU:HG2	1:J:40:LEU:N	2.27	0.49
1:B:48:HIS:HB3	1:B:51:TRP:HB2	1.95	0.49
1:H:218:ALA:HA	1:H:219:PRO:C	2.38	0.49
1:I:142:GLY:N	1:I:194:ASP:OD1	2.42	0.49
1:L:91:HIS:CG	1:L:92:PRO:HD2	2.48	0.49
1:A:166:GLU:O	1:A:167:VAL:C	2.54	0.49
1:B:87:LEU:C	1:B:87:LEU:CD2	2.86	0.49
1:C:166:GLU:O	1:C:167:VAL:C	2.56	0.49
1:J:49:PRO:O	1:J:112:VAL:HG22	2.12	0.49
1:J:165:GLU:CD	1:N:165:GLU:HB3	2.38	0.49
1:M:56:ALA:C	1:M:58:CYS:H	2.21	0.49
1:P:137:LEU:HG	1:P:138:VAL:N	2.27	0.49
1:A:48:HIS:CG	1:A:49:PRO:CD	2.96	0.48
1:C:23:SER:O	1:C:26:SER:OG	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:197:GLY:O	1:K:212:LEU:HA	2.13	0.48
1:L:98:LEU:O	1:L:99:LEU:HB2	2.11	0.48
1:M:200:ILE:HG23	1:M:208:TYR:O	2.13	0.48
1:J:48:HIS:CG	1:J:49:PRO:CD	2.96	0.48
1:J:137:LEU:HG	1:J:138:VAL:N	2.28	0.48
1:K:103:LEU:HD23	1:K:103:LEU:N	2.28	0.48
1:A:43:SER:OG	4:A:719:HOH:O	2.19	0.48
1:F:48:HIS:HB3	1:F:51:TRP:HB2	1.95	0.48
1:F:55:ALA:O	1:F:58:CYS:HB2	2.12	0.48
1:G:136:CYS:SG	1:G:201:CYS:SG	3.11	0.48
1:H:45:VAL:HG11	1:H:209:LEU:HD22	1.94	0.48
1:I:231:LEU:C	1:I:233:LYS:N	2.70	0.48
1:K:32:ALA:C	1:K:33:LEU:HD12	2.38	0.48
1:K:87:LEU:C	1:K:87:LEU:CD2	2.87	0.48
1:K:87:LEU:C	1:K:87:LEU:HD23	2.39	0.48
1:P:28:PRO:HB2	1:P:119:ARG:N	2.27	0.48
1:B:45:VAL:HG11	1:B:209:LEU:HD22	1.95	0.48
1:D:177:HIS:HB3	1:D:180:MET:HE3	1.96	0.48
1:E:28:PRO:HB2	1:E:119:ARG:N	2.27	0.48
1:E:91:HIS:CG	1:E:92:PRO:HD2	2.48	0.48
1:H:28:PRO:HB2	1:H:119:ARG:N	2.26	0.48
1:H:177:HIS:CB	1:H:180:MET:HE3	2.43	0.48
1:A:166:GLU:OE2	1:G:176:TYR:CE1	2.65	0.48
1:A:177:HIS:N	1:A:180:MET:HE3	2.29	0.48
1:B:137:LEU:HG	1:B:138:VAL:N	2.27	0.48
1:F:48:HIS:CG	1:F:49:PRO:CD	2.97	0.48
1:G:103:LEU:HB3	1:G:229:THR:HG21	1.96	0.48
1:I:231:LEU:C	1:I:233:LYS:H	2.21	0.48
1:B:123:ILE:HG12	1:B:209:LEU:HD23	1.96	0.48
1:B:170:LYS:NZ	4:B:707:HOH:O	2.31	0.48
1:D:103:LEU:HD23	1:D:103:LEU:N	2.28	0.48
1:F:48:HIS:CE1	1:F:49:PRO:HD2	2.49	0.48
1:H:48:HIS:HB3	1:H:51:TRP:HB2	1.96	0.48
1:H:231:LEU:C	1:H:233:LYS:N	2.72	0.48
1:M:23:SER:O	1:M:26:SER:OG	2.23	0.48
1:N:48:HIS:CG	1:N:49:PRO:CD	2.97	0.48
1:P:48:HIS:CG	1:P:49:PRO:CD	2.96	0.48
1:E:137:LEU:HG	1:E:138:VAL:N	2.28	0.48
1:I:23:SER:O	1:I:26:SER:OG	2.29	0.48
1:O:192:ASN:HA	3:O:715:PBZ:N1	2.28	0.48
1:A:177:HIS:HB3	1:A:180:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:PRO:HB2	1:D:119:ARG:N	2.27	0.48
1:D:48:HIS:ND1	1:D:49:PRO:HD2	2.29	0.48
1:H:23:SER:O	1:H:24:PRO:C	2.56	0.48
1:N:182:CYS:HA	1:N:226:GLY:O	2.14	0.48
1:O:197:GLY:O	1:O:212:LEU:HA	2.13	0.48
1:P:231:LEU:C	1:P:233:LYS:H	2.22	0.48
1:D:55:ALA:O	1:D:58:CYS:HB2	2.14	0.48
1:G:48:HIS:CG	1:G:49:PRO:CD	2.97	0.48
1:J:87:LEU:C	1:J:87:LEU:CD2	2.87	0.48
1:C:123:ILE:HG12	1:C:209:LEU:HD23	1.95	0.48
1:D:48:HIS:HB3	1:D:51:TRP:HB2	1.95	0.48
1:I:98:LEU:O	1:I:99:LEU:HB2	2.14	0.48
1:L:201:CYS:HB2	1:L:210:GLN:HE21	1.79	0.48
1:M:45:VAL:HG11	1:M:209:LEU:HD22	1.95	0.48
1:B:35:MET:HG2	1:B:41:PHE:CE1	2.49	0.47
1:C:158:VAL:HG22	1:C:159:ASN:N	2.29	0.47
1:F:177:HIS:N	1:F:180:MET:HE3	2.29	0.47
1:G:231:LEU:C	1:G:233:LYS:N	2.72	0.47
1:I:98:LEU:HG	1:I:99:LEU:HG	1.96	0.47
1:I:186(A):GLN:HG2	1:J:57:HIS:CD2	2.49	0.47
1:A:45:VAL:HG11	1:A:209:LEU:HD22	1.95	0.47
1:E:23:SER:O	1:E:24:PRO:C	2.55	0.47
1:G:48:HIS:CE1	1:G:49:PRO:HD2	2.49	0.47
1:J:177:HIS:HB3	1:J:180:MET:HE3	1.96	0.47
1:J:231:LEU:O	1:J:233:LYS:N	2.47	0.47
1:K:59:PHE:O	1:K:60:GLN:NE2	2.46	0.47
1:L:123:ILE:HG12	1:L:209:LEU:HD23	1.95	0.47
1:M:54:SER:OG	1:M:55:ALA:N	2.45	0.47
1:O:78:PRO:O	1:O:80:SER:N	2.47	0.47
1:D:73:LEU:N	4:D:727:HOH:O	2.42	0.47
1:G:95:ASN:C	1:G:96:ARG:HG2	2.39	0.47
1:K:171:LEU:HD13	1:K:225:PRO:HD2	1.97	0.47
1:L:197:GLY:O	1:L:212:LEU:HA	2.13	0.47
1:N:59:PHE:CB	1:N:90:ARG:HD3	2.43	0.47
1:E:49:PRO:O	1:E:112:VAL:HG22	2.14	0.47
1:J:91:HIS:O	1:J:92:PRO:C	2.57	0.47
1:P:91:HIS:O	1:P:92:PRO:C	2.58	0.47
1:B:28:PRO:HB2	1:B:119:ARG:N	2.26	0.47
1:B:231:LEU:C	1:B:233:LYS:N	2.71	0.47
1:C:87:LEU:C	1:C:87:LEU:CD2	2.87	0.47
1:D:137:LEU:HG	1:D:138:VAL:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:PHE:CB	1:E:90:ARG:HD3	2.44	0.47
1:E:191:CYS:SG	1:E:192:ASN:N	2.87	0.47
1:J:146:ASN:OD1	1:J:150:ARG:HB2	2.13	0.47
1:J:171:LEU:HD13	1:J:225:PRO:HD2	1.97	0.47
1:K:186(A):GLN:HE22	1:L:215:PHE:HB3	1.78	0.47
1:M:87:LEU:C	1:M:87:LEU:CD2	2.87	0.47
1:N:200:ILE:HA	1:N:208:TYR:O	2.14	0.47
1:O:78:PRO:C	1:O:80:SER:H	2.23	0.47
1:O:171:LEU:HD13	1:O:225:PRO:HD2	1.95	0.47
1:P:177:HIS:CB	1:P:180:MET:HE3	2.44	0.47
1:E:231:LEU:C	1:E:233:LYS:N	2.72	0.47
1:F:142:GLY:N	1:F:194:ASP:OD1	2.42	0.47
1:A:123:ILE:HG12	1:A:209:LEU:HD23	1.97	0.47
1:A:231:LEU:C	1:A:233:LYS:H	2.23	0.47
1:B:123:ILE:HA	1:B:209:LEU:HB3	1.97	0.47
1:C:35:MET:HB3	1:C:36:GLU:H	1.48	0.47
1:G:27:GLN:CA	4:G:719:HOH:O	2.62	0.47
1:G:243:GLN:HG2	1:K:243:GLN:CB	2.28	0.47
1:I:45:VAL:HG11	1:I:209:LEU:HD22	1.97	0.47
1:I:200:ILE:HA	1:I:208:TYR:O	2.15	0.47
1:J:103:LEU:HD23	1:J:103:LEU:N	2.29	0.47
1:L:22:CYS:SG	1:L:155:LEU:O	2.72	0.47
1:M:48:HIS:CE1	1:M:49:PRO:HD2	2.50	0.47
1:O:45:VAL:HG11	1:O:209:LEU:HD22	1.97	0.47
1:P:23:SER:O	1:P:26:SER:OG	2.30	0.47
1:P:103:LEU:HD23	1:P:103:LEU:N	2.28	0.47
1:A:197:GLY:O	1:A:212:LEU:HA	2.14	0.47
1:A:200:ILE:HA	1:A:208:TYR:O	2.15	0.47
1:D:123:ILE:HG12	1:D:209:LEU:HD23	1.96	0.47
1:G:91:HIS:CG	1:G:92:PRO:HD2	2.49	0.47
1:K:91:HIS:O	1:K:92:PRO:C	2.57	0.47
1:L:54:SER:OG	1:L:55:ALA:N	2.47	0.47
1:M:35:MET:HB3	1:M:36:GLU:H	1.46	0.47
1:O:48:HIS:HB3	1:O:51:TRP:HB2	1.96	0.47
1:A:171:LEU:HD13	1:A:225:PRO:HD2	1.95	0.47
1:A:201:CYS:CB	1:A:210:GLN:HE21	2.26	0.47
1:B:95:ASN:C	1:B:96:ARG:HG2	2.39	0.47
1:B:97:PRO:O	1:B:98:LEU:C	2.58	0.47
1:G:48:HIS:ND1	1:G:49:PRO:N	2.62	0.47
1:I:140:GLY:CA	4:I:723:HOH:O	2.63	0.47
1:O:28:PRO:HB2	1:O:119:ARG:N	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:98:LEU:HG	1:P:99:LEU:HG	1.97	0.47
1:B:177:HIS:HB3	1:B:180:MET:HE3	1.96	0.47
1:C:59:PHE:O	1:C:60:GLN:NE2	2.45	0.47
1:G:79:GLY:CA	4:G:714:HOH:O	2.62	0.47
1:J:48:HIS:CE1	1:J:49:PRO:HD2	2.49	0.47
1:O:59:PHE:O	1:O:60:GLN:NE2	2.48	0.47
1:P:171:LEU:HD13	1:P:225:PRO:HD2	1.97	0.47
1:P:177:HIS:N	1:P:180:MET:HE3	2.30	0.47
1:P:181:PHE:HZ	1:P:199:LEU:HD23	1.79	0.47
1:D:176:TYR:CE1	1:H:166:GLU:OE2	2.66	0.46
1:F:231:LEU:C	1:F:233:LYS:N	2.72	0.46
1:G:171:LEU:HD13	1:G:225:PRO:HD2	1.95	0.46
1:H:129:PRO:HA	4:H:719:HOH:O	2.14	0.46
1:L:93:GLU:O	1:L:94:TYR:C	2.54	0.46
1:M:136:CYS:HB3	1:M:200:ILE:O	2.15	0.46
1:M:201:CYS:HB2	1:M:210:GLN:HE21	1.81	0.46
1:N:192:ASN:OD1	3:N:714:PBZ:H2	2.15	0.46
1:O:123:ILE:HG12	1:O:209:LEU:HD23	1.96	0.46
1:D:48:HIS:CG	1:D:49:PRO:CD	2.99	0.46
1:D:56:ALA:C	1:D:58:CYS:H	2.22	0.46
1:E:95:ASN:C	1:E:96:ARG:HG2	2.40	0.46
1:F:95:ASN:C	1:F:96:ARG:HG2	2.38	0.46
1:F:137:LEU:HG	1:F:138:VAL:N	2.28	0.46
1:G:93:GLU:O	1:G:94:TYR:C	2.53	0.46
1:G:98:LEU:HG	1:G:99:LEU:HG	1.96	0.46
1:I:141:TRP:N	4:I:723:HOH:O	2.27	0.46
1:P:32:ALA:C	1:P:33:LEU:HD12	2.40	0.46
1:B:201:CYS:HB2	1:B:210:GLN:NE2	2.24	0.46
1:C:91:HIS:CG	1:C:92:PRO:HD2	2.50	0.46
1:E:35:MET:HB3	1:E:36:GLU:H	1.45	0.46
1:E:48:HIS:ND1	1:E:49:PRO:HD2	2.29	0.46
1:E:175:LEU:HA	1:E:175:LEU:HD23	1.66	0.46
1:E:197:GLY:O	1:E:212:LEU:HA	2.15	0.46
1:F:28:PRO:HB2	1:F:119:ARG:N	2.28	0.46
1:I:93:GLU:O	1:I:94:TYR:C	2.56	0.46
1:I:166:GLU:O	1:I:167:VAL:C	2.57	0.46
1:L:48:HIS:CG	1:L:49:PRO:CD	2.98	0.46
1:M:61:ASN:ND2	4:M:739:HOH:O	2.47	0.46
1:M:158:VAL:HG22	1:M:159:ASN:N	2.31	0.46
1:A:175:LEU:HA	1:A:175:LEU:HD23	1.67	0.46
1:B:103:LEU:HB3	1:B:229:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:VAL:HG22	1:H:159:ASN:N	2.30	0.46
1:J:69:GLY:CA	1:J:118:ILE:HG12	2.46	0.46
1:M:137:LEU:HD11	1:M:157:CYS:HB3	1.97	0.46
1:N:123:ILE:HA	1:N:209:LEU:HB3	1.97	0.46
1:O:142:GLY:N	1:O:194:ASP:OD1	2.45	0.46
1:B:23:SER:O	1:B:26:SER:OG	2.32	0.46
1:E:48:HIS:CG	1:E:49:PRO:CD	2.98	0.46
1:E:93:GLU:O	1:E:94:TYR:C	2.56	0.46
1:E:98:LEU:O	1:E:99:LEU:HB2	2.15	0.46
1:I:123:ILE:HG12	1:I:209:LEU:HD23	1.97	0.46
1:I:171:LEU:HD13	1:I:225:PRO:HD2	1.97	0.46
1:J:48:HIS:HB3	1:J:51:TRP:HB2	1.96	0.46
1:M:91:HIS:O	1:M:92:PRO:C	2.55	0.46
1:M:91:HIS:CG	1:M:92:PRO:HD2	2.51	0.46
1:B:50:GLN:HG3	1:B:111:SER:CA	2.45	0.46
1:C:48:HIS:HB3	1:C:51:TRP:HB2	1.96	0.46
1:C:103:LEU:HB3	1:C:229:THR:HG21	1.97	0.46
1:F:103:LEU:HD23	1:F:103:LEU:N	2.28	0.46
1:H:123:ILE:HA	1:H:209:LEU:HB3	1.96	0.46
1:H:166:GLU:O	1:H:167:VAL:C	2.54	0.46
1:J:23:SER:O	1:J:24:PRO:C	2.56	0.46
1:N:54:SER:OG	1:N:55:ALA:N	2.46	0.46
1:O:23:SER:O	1:O:26:SER:OG	2.31	0.46
1:P:48:HIS:HB3	1:P:51:TRP:HB2	1.98	0.46
1:P:59:PHE:O	1:P:60:GLN:NE2	2.47	0.46
1:P:123:ILE:HG12	1:P:209:LEU:HD23	1.98	0.46
1:P:231:LEU:C	1:P:233:LYS:N	2.70	0.46
1:A:146:ASN:OD1	1:A:150:ARG:HB2	2.16	0.46
1:C:231:LEU:C	1:C:233:LYS:N	2.73	0.46
1:D:50:GLN:HG3	1:D:111:SER:CA	2.45	0.46
1:D:59:PHE:CB	1:D:90:ARG:HD3	2.46	0.46
1:F:182:CYS:HA	1:F:226:GLY:O	2.16	0.46
1:H:98:LEU:O	1:H:99:LEU:HB2	2.16	0.46
1:I:189:ASP:CG	1:I:190:SER:N	2.74	0.46
1:J:189:ASP:CG	1:J:190:SER:N	2.73	0.46
1:D:23:SER:O	1:D:24:PRO:C	2.59	0.46
1:D:87:LEU:C	1:D:87:LEU:HD23	2.40	0.46
1:F:59:PHE:CB	1:F:90:ARG:HD3	2.46	0.46
1:H:59:PHE:O	1:H:60:GLN:NE2	2.48	0.46
1:H:91:HIS:CG	1:H:92:PRO:HD2	2.51	0.46
1:I:59:PHE:CB	1:I:90:ARG:HD3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:48:HIS:ND1	1:K:49:PRO:HD2	2.31	0.46
1:K:123:ILE:HG12	1:K:209:LEU:HD23	1.97	0.46
1:K:177:HIS:CB	1:K:180:MET:HE3	2.45	0.46
1:P:166:GLU:O	1:P:167:VAL:C	2.56	0.46
1:B:23:SER:O	1:B:24:PRO:C	2.59	0.46
1:D:215:PHE:HA	3:D:704:PBZ:H6	1.97	0.46
1:G:69:GLY:CA	1:G:118:ILE:HG12	2.46	0.46
1:H:29:TRP:CE3	1:H:121:ILE:HB	2.50	0.46
1:L:22:CYS:SG	1:L:155:LEU:HG	2.56	0.46
1:P:35:MET:HB3	1:P:36:GLU:H	1.46	0.46
1:A:190:SER:O	1:A:191:CYS:HB2	2.16	0.46
1:F:54:SER:OG	1:F:55:ALA:N	2.49	0.46
1:M:23:SER:O	1:M:24:PRO:C	2.58	0.46
1:M:95:ASN:C	1:M:96:ARG:HG2	2.41	0.46
1:M:197:GLY:O	1:M:212:LEU:HA	2.16	0.46
1:P:189:ASP:CG	1:P:190:SER:N	2.73	0.46
1:A:231:LEU:O	1:A:232:CYS:C	2.54	0.45
1:F:171:LEU:HD13	1:F:225:PRO:HD2	1.98	0.45
1:M:123:ILE:HG12	1:M:209:LEU:HD23	1.98	0.45
1:B:49:PRO:O	1:B:112:VAL:HG22	2.16	0.45
1:C:48:HIS:CE1	1:C:49:PRO:HD2	2.51	0.45
1:D:158:VAL:HG22	1:D:159:ASN:N	2.31	0.45
1:E:23:SER:O	1:E:26:SER:OG	2.29	0.45
1:E:123:ILE:HG12	1:E:209:LEU:HD23	1.98	0.45
1:F:91:HIS:CG	1:F:92:PRO:HD2	2.51	0.45
1:I:69:GLY:CA	1:I:118:ILE:HG12	2.47	0.45
1:M:171:LEU:HD13	1:M:225:PRO:HD2	1.99	0.45
1:M:186(A):GLN:HG2	1:N:57:HIS:CD2	2.51	0.45
1:O:137:LEU:HG	1:O:138:VAL:N	2.31	0.45
1:P:220:CYS:SG	3:P:716:PBZ:H5	2.56	0.45
1:E:128:CYS:O	1:E:129:PRO:C	2.57	0.45
1:F:158:VAL:HG22	1:F:159:ASN:N	2.32	0.45
1:K:128:CYS:HB3	1:K:129:PRO:HD2	1.98	0.45
1:M:48:HIS:CG	1:M:49:PRO:CD	2.99	0.45
1:A:208:TYR:HE2	4:A:703:HOH:O	1.99	0.45
1:C:95:ASN:C	1:C:96:ARG:HG2	2.39	0.45
1:C:186(A):GLN:HE22	1:D:215:PHE:HB3	1.81	0.45
1:E:32:ALA:C	1:E:33:LEU:HD12	2.41	0.45
1:F:78:PRO:C	1:F:80:SER:N	2.75	0.45
1:H:137:LEU:HG	1:H:138:VAL:N	2.31	0.45
1:H:171:LEU:HD13	1:H:225:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:123:ILE:HA	1:J:209:LEU:HB3	1.98	0.45
1:L:59:PHE:CB	1:L:90:ARG:HD3	2.46	0.45
1:L:103:LEU:HD23	1:L:103:LEU:N	2.31	0.45
1:M:48:HIS:HB3	1:M:51:TRP:HB2	1.98	0.45
1:M:142:GLY:N	1:M:194:ASP:OD1	2.44	0.45
1:N:136:CYS:O	1:N:159:ASN:HA	2.16	0.45
1:N:171:LEU:HD13	1:N:225:PRO:HD2	1.98	0.45
1:E:243:GLN:HB3	1:E:244:ALA:H	1.62	0.45
1:F:175:LEU:HD23	1:F:175:LEU:HA	1.71	0.45
1:G:23:SER:O	1:G:24:PRO:C	2.59	0.45
1:M:97:PRO:O	1:M:98:LEU:C	2.60	0.45
1:M:177:HIS:HB3	1:M:180:MET:HE3	1.97	0.45
1:C:189:ASP:CG	1:C:190:SER:N	2.75	0.45
1:D:87:LEU:C	1:D:87:LEU:CD2	2.89	0.45
1:F:69:GLY:CA	1:F:118:ILE:HG12	2.46	0.45
1:M:98:LEU:O	1:M:99:LEU:HB2	2.17	0.45
1:N:142:GLY:N	1:N:194:ASP:OD1	2.45	0.45
1:A:48:HIS:CE1	1:A:49:PRO:HD2	2.52	0.45
1:C:69:GLY:CA	1:C:118:ILE:HG12	2.47	0.45
1:D:69:GLY:CA	1:D:118:ILE:HG12	2.47	0.45
1:G:48:HIS:HB3	1:G:51:TRP:HB2	1.97	0.45
1:H:163:VAL:HB	1:H:182:CYS:HB2	1.97	0.45
1:I:23:SER:O	1:I:24:PRO:C	2.60	0.45
1:J:179:SER:HB2	1:J:234:PHE:HZ	1.82	0.45
1:K:201:CYS:HB2	1:K:210:GLN:HE21	1.82	0.45
1:L:177:HIS:CD2	1:L:179:SER:H	2.34	0.45
1:M:189:ASP:CG	1:M:190:SER:N	2.75	0.45
1:N:146:ASN:OD1	1:N:150:ARG:HB2	2.17	0.45
1:B:171:LEU:HD13	1:B:225:PRO:HD2	1.99	0.45
1:B:201:CYS:O	1:B:202:ASN:HB2	2.17	0.45
1:E:103:LEU:HD23	1:E:103:LEU:N	2.32	0.45
1:G:32:ALA:C	1:G:33:LEU:HD12	2.42	0.45
1:M:49:PRO:O	1:M:112:VAL:HG22	2.17	0.45
1:M:103:LEU:HD23	1:M:103:LEU:H	1.82	0.45
1:M:220:CYS:SG	3:M:713:PBZ:H3	2.56	0.45
1:N:177:HIS:HB3	1:N:180:MET:HE3	1.97	0.45
1:O:146:ASN:OD1	1:O:150:ARG:HB2	2.16	0.45
1:P:127:GLN:HB2	4:P:733:HOH:O	2.17	0.45
1:A:78:PRO:C	1:A:80:SER:N	2.75	0.45
1:C:23:SER:O	1:C:24:PRO:C	2.58	0.45
1:C:59:PHE:CB	1:C:90:ARG:HD3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:GLU:O	1:D:94:TYR:C	2.57	0.45
1:H:192:ASN:CG	3:H:708:PBZ:H6	2.42	0.45
1:I:48:HIS:ND1	1:I:49:PRO:HD2	2.31	0.45
1:N:137:LEU:HG	1:N:138:VAL:N	2.30	0.45
1:O:91:HIS:CG	1:O:92:PRO:HD2	2.52	0.45
1:A:57:HIS:CG	1:D:186(A):GLN:HG2	2.51	0.45
1:A:231:LEU:O	1:A:233:LYS:N	2.50	0.45
1:B:69:GLY:CA	1:B:118:ILE:HG12	2.47	0.45
1:B:186(A):GLN:HE22	1:C:215:PHE:HB2	1.77	0.45
1:C:171:LEU:HD13	1:C:225:PRO:HD2	1.99	0.45
1:E:200:ILE:HA	1:E:208:TYR:O	2.17	0.45
1:I:57:HIS:CD2	1:L:186(A):GLN:HG2	2.52	0.45
1:K:54:SER:OG	1:K:55:ALA:N	2.51	0.45
1:N:91:HIS:CG	1:N:92:PRO:HD2	2.52	0.45
1:P:48:HIS:CE1	1:P:49:PRO:HD2	2.52	0.45
1:P:59:PHE:CB	1:P:90:ARG:HD3	2.47	0.45
1:P:201:CYS:HB2	1:P:210:GLN:HE21	1.82	0.45
1:B:48:HIS:ND1	1:B:49:PRO:CD	2.80	0.44
1:B:59:PHE:CB	1:B:90:ARG:HD3	2.46	0.44
1:B:201:CYS:CB	1:B:210:GLN:HE21	2.24	0.44
1:E:29:TRP:CE3	1:E:121:ILE:HB	2.53	0.44
1:E:166:GLU:O	1:E:167:VAL:C	2.59	0.44
1:E:195:SER:OG	3:E:705:PBZ:N1	2.39	0.44
1:F:45:VAL:HG11	1:F:209:LEU:HD22	1.97	0.44
1:G:158:VAL:HG22	1:G:159:ASN:N	2.32	0.44
1:H:69:GLY:CA	1:H:118:ILE:HG12	2.47	0.44
1:I:95:ASN:C	1:I:96:ARG:HG2	2.42	0.44
1:J:54:SER:OG	1:J:55:ALA:N	2.50	0.44
1:K:35:MET:HB3	1:K:36:GLU:H	1.49	0.44
1:N:48:HIS:CE1	1:N:49:PRO:HD2	2.52	0.44
1:O:48:HIS:ND1	1:O:49:PRO:HD2	2.32	0.44
1:E:112:VAL:HA	4:E:714:HOH:O	2.17	0.44
1:E:231:LEU:O	1:E:232:CYS:C	2.53	0.44
1:F:189:ASP:CG	1:F:190:SER:N	2.75	0.44
1:M:137:LEU:HG	1:M:138:VAL:N	2.31	0.44
1:O:231:LEU:C	1:O:233:LYS:N	2.75	0.44
1:B:48:HIS:ND1	1:B:49:PRO:N	2.66	0.44
1:B:181:PHE:HZ	1:B:199:LEU:HD23	1.83	0.44
1:C:50:GLN:HG3	1:C:111:SER:CA	2.47	0.44
1:D:197:GLY:O	1:D:212:LEU:HA	2.16	0.44
1:L:23:SER:O	1:L:26:SER:OG	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:87:LEU:C	1:L:87:LEU:CD2	2.90	0.44
1:L:87:LEU:C	1:L:87:LEU:HD23	2.42	0.44
1:M:177:HIS:N	1:M:180:MET:HE3	2.32	0.44
1:N:59:PHE:O	1:N:60:GLN:NE2	2.50	0.44
1:C:48:HIS:CG	1:C:49:PRO:CD	3.00	0.44
1:E:220:CYS:SG	3:E:705:PBZ:N3	2.90	0.44
1:G:59:PHE:CB	1:G:90:ARG:HD3	2.46	0.44
1:H:95:ASN:C	1:H:96:ARG:HG2	2.42	0.44
1:J:59:PHE:CB	1:J:90:ARG:HD3	2.47	0.44
1:K:50:GLN:HG3	1:K:111:SER:CA	2.48	0.44
1:L:181:PHE:HZ	1:L:199:LEU:HD23	1.82	0.44
1:N:45:VAL:HG11	1:N:209:LEU:HD22	1.99	0.44
1:N:231:LEU:C	1:N:233:LYS:H	2.25	0.44
1:P:78:PRO:C	1:P:80:SER:N	2.74	0.44
1:A:93:GLU:O	1:A:94:TYR:C	2.60	0.44
1:B:32:ALA:C	1:B:33:LEU:HD12	2.42	0.44
1:D:95:ASN:C	1:D:96:ARG:HG2	2.42	0.44
1:G:177:HIS:N	1:G:180:MET:HE3	2.32	0.44
1:H:189:ASP:CG	1:H:190:SER:N	2.76	0.44
1:I:181:PHE:HZ	1:I:199:LEU:HD23	1.83	0.44
1:J:93:GLU:O	1:J:94:TYR:C	2.57	0.44
1:K:103:LEU:HB3	1:K:229:THR:HG21	2.00	0.44
1:N:48:HIS:HB3	1:N:51:TRP:HB2	1.99	0.44
1:P:158:VAL:HG22	1:P:159:ASN:N	2.32	0.44
1:A:95:ASN:C	1:A:96:ARG:HG2	2.43	0.44
1:A:163:VAL:HG12	1:A:164:SER:N	2.31	0.44
1:C:181:PHE:HZ	1:C:199:LEU:HD23	1.82	0.44
1:G:98:LEU:O	1:G:99:LEU:HB2	2.17	0.44
1:I:49:PRO:O	1:I:112:VAL:HG22	2.18	0.44
1:I:200:ILE:HG23	1:I:208:TYR:O	2.18	0.44
1:M:32:ALA:C	1:M:33:LEU:HD12	2.43	0.44
1:O:158:VAL:HG22	1:O:159:ASN:N	2.33	0.44
1:A:103:LEU:HD23	1:A:103:LEU:N	2.33	0.44
1:A:180:MET:HB2	1:A:227:VAL:CG1	2.47	0.44
1:E:35:MET:HG2	1:E:41:PHE:CD1	2.53	0.44
1:F:35:MET:HB3	1:F:36:GLU:H	1.43	0.44
1:G:231:LEU:C	1:G:233:LYS:H	2.25	0.44
1:G:243:GLN:CG	1:K:244:ALA:HB2	2.34	0.44
1:H:54:SER:OG	1:H:55:ALA:N	2.49	0.44
1:H:177:HIS:N	1:H:180:MET:HE3	2.33	0.44
1:J:158:VAL:HG22	1:J:159:ASN:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:175:LEU:HD23	1:J:175:LEU:HA	1.76	0.44
1:K:69:GLY:CA	1:K:118:ILE:HG12	2.48	0.44
1:L:19:GLY:HA3	1:L:157:CYS:O	2.17	0.44
1:M:93:GLU:O	1:M:94:TYR:C	2.57	0.44
1:N:158:VAL:HG22	1:N:159:ASN:N	2.32	0.44
1:O:21:ASP:C	1:O:22:CYS:O	2.59	0.44
1:O:200:ILE:HA	1:O:208:TYR:O	2.18	0.44
1:A:32:ALA:C	1:A:33:LEU:HD12	2.42	0.44
1:C:123:ILE:HA	1:C:209:LEU:HB3	2.00	0.44
1:D:32:ALA:C	1:D:33:LEU:HD12	2.43	0.44
1:I:177:HIS:CE1	4:I:728:HOH:O	2.68	0.44
1:J:29:TRP:CE3	1:J:121:ILE:HB	2.53	0.44
1:L:35:MET:HG2	1:L:41:PHE:CD1	2.53	0.44
1:L:69:GLY:CA	1:L:118:ILE:HG12	2.48	0.44
1:P:175:LEU:HA	1:P:175:LEU:HD23	1.71	0.44
1:C:48:HIS:ND1	1:C:49:PRO:N	2.66	0.44
1:H:175:LEU:HD23	1:H:175:LEU:HA	1.74	0.44
1:K:97:PRO:O	1:K:98:LEU:C	2.61	0.44
1:M:28:PRO:HB2	1:M:119:ARG:N	2.30	0.44
1:N:49:PRO:O	1:N:112:VAL:HG22	2.18	0.44
1:O:139:SER:HA	1:O:156:GLN:O	2.18	0.44
1:O:243:GLN:HB3	1:O:244:ALA:H	1.64	0.44
1:B:201:CYS:O	1:B:202:ASN:C	2.59	0.43
1:D:48:HIS:CE1	1:D:49:PRO:HD2	2.53	0.43
1:F:200:ILE:HA	1:F:208:TYR:O	2.18	0.43
1:G:48:HIS:ND1	1:G:49:PRO:CD	2.80	0.43
1:I:78:PRO:C	1:I:80:SER:N	2.76	0.43
1:J:42:CYS:HB3	1:J:43:SER:H	1.61	0.43
1:J:48:HIS:ND1	1:J:49:PRO:CD	2.81	0.43
1:J:111:SER:N	4:J:731:HOH:O	2.45	0.43
1:J:165:GLU:HB3	1:N:165:GLU:CD	2.43	0.43
1:K:189:ASP:CG	1:K:190:SER:N	2.76	0.43
1:L:32:ALA:C	1:L:33:LEU:HD12	2.43	0.43
1:L:49:PRO:O	1:L:112:VAL:HG22	2.18	0.43
1:N:175:LEU:HD23	1:N:175:LEU:HA	1.72	0.43
1:N:231:LEU:C	1:N:233:LYS:N	2.74	0.43
1:O:35:MET:HB3	1:O:36:GLU:H	1.49	0.43
1:O:59:PHE:CB	1:O:90:ARG:HD3	2.48	0.43
1:O:189:ASP:CG	1:O:190:SER:N	2.76	0.43
1:P:48:HIS:ND1	1:P:49:PRO:N	2.65	0.43
1:A:159:ASN:HB3	1:K:116:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:LEU:HD13	1:D:225:PRO:HD2	2.00	0.43
1:D:190:SER:O	3:D:704:PBZ:N2	2.50	0.43
1:F:123:ILE:HA	1:F:209:LEU:HB3	1.99	0.43
1:G:97:PRO:O	1:G:98:LEU:C	2.61	0.43
1:G:123:ILE:HA	1:G:209:LEU:HB3	2.00	0.43
1:I:175:LEU:HD23	1:I:175:LEU:HA	1.68	0.43
1:K:48:HIS:CG	1:K:49:PRO:CD	3.01	0.43
1:L:48:HIS:ND1	1:L:49:PRO:N	2.66	0.43
1:M:59:PHE:CB	1:M:90:ARG:HD3	2.48	0.43
1:N:28:PRO:HB2	1:N:119:ARG:N	2.29	0.43
1:P:54:SER:OG	1:P:55:ALA:N	2.51	0.43
1:P:203:GLY:HA2	4:P:720:HOH:O	2.18	0.43
1:A:97:PRO:O	1:A:98:LEU:C	2.61	0.43
1:G:35:MET:HG2	1:G:41:PHE:CD1	2.54	0.43
1:I:166:GLU:OE2	1:O:176:TYR:HE1	2.02	0.43
1:L:35:MET:HB3	1:L:36:GLU:H	1.52	0.43
1:B:40:LEU:C	1:B:40:LEU:CD1	2.91	0.43
1:B:177:HIS:N	1:B:180:MET:HE3	2.34	0.43
1:F:48:HIS:ND1	1:F:49:PRO:CD	2.82	0.43
1:F:201:CYS:O	1:F:202:ASN:HB2	2.18	0.43
1:J:45:VAL:HG11	1:J:209:LEU:HD22	2.00	0.43
1:N:166:GLU:O	1:N:167:VAL:C	2.58	0.43
1:O:191:CYS:HA	3:O:715:PBZ:C3	2.48	0.43
1:P:59:PHE:CD2	1:P:60:GLN:N	2.86	0.43
1:P:93:GLU:O	1:P:94:TYR:C	2.58	0.43
1:P:121:ILE:CG1	1:P:122:SER:N	2.81	0.43
1:A:53:LEU:HD12	1:A:53:LEU:HA	1.77	0.43
1:A:158:VAL:HG22	1:A:159:ASN:N	2.33	0.43
1:C:29:TRP:CE3	1:C:121:ILE:HB	2.53	0.43
1:C:200:ILE:HA	1:C:208:TYR:O	2.17	0.43
1:D:190:SER:HB2	3:D:704:PBZ:N2	2.25	0.43
1:E:181:PHE:HZ	1:E:199:LEU:HD23	1.83	0.43
1:F:48:HIS:ND1	1:F:49:PRO:N	2.66	0.43
1:F:91:HIS:O	1:F:92:PRO:C	2.61	0.43
1:G:54:SER:OG	1:G:55:ALA:N	2.51	0.43
1:H:35:MET:HG2	1:H:41:PHE:CD1	2.53	0.43
1:J:59:PHE:O	1:J:60:GLN:NE2	2.51	0.43
1:J:201:CYS:HB2	1:J:210:GLN:HE21	1.84	0.43
1:L:137:LEU:HG	1:L:138:VAL:N	2.33	0.43
1:M:200:ILE:HA	1:M:208:TYR:O	2.18	0.43
1:N:93:GLU:O	1:N:94:TYR:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:95:ASN:C	1:P:96:ARG:HG2	2.43	0.43
1:A:191:CYS:O	1:A:192:ASN:C	2.58	0.43
1:B:166:GLU:O	1:B:167:VAL:C	2.59	0.43
1:H:177:HIS:CD2	1:H:179:SER:H	2.37	0.43
1:L:48:HIS:CE1	1:L:49:PRO:HD2	2.54	0.43
1:N:35:MET:HB3	1:N:36:GLU:H	1.47	0.43
1:N:122:SER:CB	4:N:721:HOH:O	2.66	0.43
1:O:48:HIS:CG	1:O:49:PRO:CD	3.02	0.43
1:O:69:GLY:CA	1:O:118:ILE:HG12	2.49	0.43
1:O:123:ILE:HA	1:O:209:LEU:HB3	1.99	0.43
1:O:181:PHE:HZ	1:O:199:LEU:HD23	1.82	0.43
1:B:91:HIS:CG	1:B:92:PRO:HD2	2.54	0.43
1:C:78:PRO:C	1:C:80:SER:N	2.77	0.43
1:G:123:ILE:HG12	1:G:209:LEU:HD23	1.99	0.43
3:H:708:PBZ:N1	4:H:710:HOH:O	2.37	0.43
1:I:22:CYS:HB2	1:I:155:LEU:O	2.18	0.43
1:I:137:LEU:HG	1:I:138:VAL:N	2.32	0.43
1:J:91:HIS:CG	1:J:92:PRO:HD2	2.54	0.43
1:N:69:GLY:CA	1:N:118:ILE:HG12	2.49	0.43
1:A:69:GLY:CA	1:A:118:ILE:HG12	2.49	0.43
1:C:103:LEU:HD23	1:C:103:LEU:N	2.31	0.43
1:D:181:PHE:HZ	1:D:199:LEU:HD23	1.82	0.43
1:E:69:GLY:CA	1:E:118:ILE:HG12	2.49	0.43
1:H:23:SER:O	1:H:26:SER:OG	2.32	0.43
1:M:40:LEU:C	1:M:40:LEU:CD1	2.92	0.43
1:N:95:ASN:C	1:N:96:ARG:HG2	2.43	0.43
1:P:70:LEU:N	4:P:727:HOH:O	2.30	0.43
1:B:186(A):GLN:NE2	1:C:215:PHE:HB3	2.32	0.43
1:E:123:ILE:HA	1:E:209:LEU:HB3	2.01	0.43
1:E:171:LEU:HD13	1:E:225:PRO:HD2	2.01	0.43
1:G:79:GLY:HA3	4:G:714:HOH:O	2.19	0.43
1:I:33:LEU:O	1:I:40:LEU:HD22	2.19	0.43
1:J:103:LEU:HB3	1:J:229:THR:HG21	2.01	0.43
1:P:22:CYS:SG	1:P:156:GLN:C	3.02	0.43
1:P:69:GLY:CA	1:P:118:ILE:HG12	2.49	0.43
1:A:23:SER:O	1:A:24:PRO:C	2.62	0.43
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.73	0.43
1:C:231:LEU:C	1:C:233:LYS:H	2.26	0.43
1:D:49:PRO:O	1:D:112:VAL:HG22	2.19	0.43
1:E:189:ASP:CG	1:E:190:SER:N	2.77	0.43
1:G:59:PHE:O	1:G:60:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:GLN:CD	1:K:240:LYS:HA	2.43	0.43
1:I:54:SER:OG	1:I:55:ALA:N	2.51	0.43
1:J:182:CYS:HA	1:J:226:GLY:O	2.18	0.43
1:J:200:ILE:HA	1:J:208:TYR:O	2.19	0.43
1:K:78:PRO:C	1:K:80:SER:N	2.77	0.43
1:O:87:LEU:C	1:O:87:LEU:CD2	2.92	0.43
1:C:144:LEU:HB2	1:C:146:ASN:OD1	2.19	0.42
1:F:180:MET:HB2	1:F:227:VAL:CG1	2.49	0.42
1:I:32:ALA:C	1:I:33:LEU:HD12	2.43	0.42
1:I:103:LEU:HB3	1:I:229:THR:HG21	2.00	0.42
1:K:59:PHE:CB	1:K:90:ARG:HD3	2.47	0.42
1:K:158:VAL:HG22	1:K:159:ASN:N	2.33	0.42
1:K:175:LEU:HD23	1:K:175:LEU:HA	1.73	0.42
1:A:54:SER:OG	1:A:55:ALA:N	2.52	0.42
1:B:103:LEU:HD23	1:B:103:LEU:N	2.33	0.42
1:C:175:LEU:HA	1:C:175:LEU:HD23	1.74	0.42
1:I:48:HIS:CG	1:I:49:PRO:CD	3.02	0.42
1:K:182:CYS:N	4:K:714:HOH:O	2.36	0.42
1:L:91:HIS:O	1:L:92:PRO:C	2.62	0.42
1:L:171:LEU:HD13	1:L:225:PRO:HD2	2.01	0.42
1:O:177:HIS:CB	1:O:180:MET:HE3	2.48	0.42
1:P:78:PRO:HA	4:P:735:HOH:O	2.12	0.42
1:H:139:SER:HA	1:H:156:GLN:O	2.19	0.42
1:K:95:ASN:C	1:K:96:ARG:HG2	2.43	0.42
1:L:128:CYS:HB3	1:L:129:PRO:CD	2.50	0.42
1:B:165:GLU:HB3	1:F:165:GLU:HB3	2.01	0.42
1:D:166:GLU:O	1:D:167:VAL:C	2.60	0.42
1:F:177:HIS:CB	1:F:180:MET:HE3	2.49	0.42
1:G:69:GLY:N	1:G:118:ILE:HG12	2.34	0.42
1:I:180:MET:HB2	1:I:227:VAL:CG1	2.49	0.42
1:J:48:HIS:ND1	1:J:49:PRO:N	2.67	0.42
1:L:123:ILE:HA	1:L:209:LEU:HB3	2.00	0.42
1:M:35:MET:HG2	1:M:41:PHE:CD1	2.54	0.42
1:O:91:HIS:O	1:O:92:PRO:C	2.61	0.42
1:P:50:GLN:HG3	1:P:111:SER:CA	2.50	0.42
1:P:215:PHE:HB2	4:P:728:HOH:O	2.18	0.42
1:C:177:HIS:N	1:C:180:MET:HE3	2.35	0.42
1:C:180:MET:HB2	1:C:227:VAL:CG1	2.50	0.42
1:G:35:MET:HB3	1:G:36:GLU:H	1.52	0.42
1:G:103:LEU:HD23	1:G:103:LEU:N	2.34	0.42
1:G:137:LEU:HG	1:G:138:VAL:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:97:PRO:O	1:I:98:LEU:C	2.62	0.42
1:M:123:ILE:HD13	1:M:238:ILE:HD13	2.01	0.42
1:A:128:CYS:HB3	1:A:129:PRO:CD	2.48	0.42
1:B:91:HIS:O	1:B:92:PRO:C	2.61	0.42
1:D:48:HIS:ND1	1:D:49:PRO:N	2.67	0.42
1:D:180:MET:HB2	1:D:227:VAL:CG1	2.50	0.42
1:K:177:HIS:N	1:K:180:MET:HE3	2.35	0.42
1:M:69:GLY:CA	1:M:118:ILE:HG12	2.49	0.42
1:M:231:LEU:C	1:M:233:LYS:N	2.73	0.42
1:O:94:TYR:HA	1:O:101:ASN:HB2	2.02	0.42
1:A:123:ILE:HA	1:A:209:LEU:HB3	2.02	0.42
1:E:158:VAL:HG22	1:E:159:ASN:N	2.34	0.42
1:E:180:MET:HB2	1:E:227:VAL:CG1	2.49	0.42
1:G:78:PRO:C	1:G:80:SER:N	2.78	0.42
1:G:91:HIS:O	1:G:92:PRO:C	2.62	0.42
1:G:215:PHE:HA	3:G:707:PBZ:C6	2.49	0.42
1:H:190:SER:O	3:H:708:PBZ:N3	2.52	0.42
1:I:50:GLN:HG3	1:I:111:SER:CA	2.50	0.42
1:J:121:ILE:CG1	1:J:122:SER:N	2.82	0.42
1:O:166:GLU:O	1:O:167:VAL:C	2.62	0.42
1:P:23:SER:O	1:P:24:PRO:C	2.61	0.42
1:A:48:HIS:ND1	1:A:49:PRO:N	2.68	0.42
1:A:137:LEU:HG	1:A:138:VAL:N	2.33	0.42
1:C:91:HIS:O	1:C:92:PRO:C	2.61	0.42
1:F:177:HIS:HB3	1:F:180:MET:CE	2.49	0.42
1:G:189:ASP:CG	1:G:190:SER:N	2.78	0.42
1:I:136:CYS:HB3	1:I:200:ILE:O	2.20	0.42
1:I:182:CYS:HA	1:I:226:GLY:O	2.20	0.42
1:J:50:GLN:HG3	1:J:111:SER:CA	2.49	0.42
1:N:136:CYS:HB3	1:N:200:ILE:O	2.19	0.42
1:O:87:LEU:C	1:O:87:LEU:HD23	2.44	0.42
1:P:33:LEU:O	1:P:40:LEU:HD22	2.20	0.42
1:B:200:ILE:HA	1:B:208:TYR:O	2.20	0.42
1:C:200:ILE:HG23	1:C:208:TYR:O	2.20	0.42
1:D:103:LEU:HB3	1:D:229:THR:HG21	2.02	0.42
1:D:175:LEU:HD23	1:D:175:LEU:HA	1.64	0.42
1:F:59:PHE:O	1:F:60:GLN:NE2	2.51	0.42
1:F:69:GLY:N	1:F:118:ILE:HG12	2.35	0.42
1:G:121:ILE:CG1	1:G:122:SER:N	2.82	0.42
1:J:35:MET:HG2	1:J:41:PHE:CD1	2.55	0.42
1:K:17:ILE:HG12	1:K:191:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:91:HIS:CG	1:P:92:PRO:HD2	2.54	0.42
1:B:35:MET:HG2	1:B:41:PHE:CD1	2.55	0.42
1:B:54:SER:OG	1:B:55:ALA:N	2.52	0.42
1:G:166:GLU:O	1:G:167:VAL:C	2.62	0.42
1:I:29:TRP:CE3	1:I:121:ILE:HB	2.54	0.42
1:L:22:CYS:SG	1:L:156:GLN:C	3.02	0.42
1:O:180:MET:HB2	1:O:227:VAL:CG1	2.50	0.42
1:D:231:LEU:O	1:D:233:LYS:N	2.53	0.41
1:E:103:LEU:HB3	1:E:229:THR:HG21	2.02	0.41
1:G:177:HIS:CD2	1:G:179:SER:H	2.38	0.41
1:H:32:ALA:C	1:H:33:LEU:HD12	2.45	0.41
1:I:179:SER:HB2	1:I:234:PHE:HZ	1.84	0.41
1:N:243:GLN:HB3	1:N:244:ALA:H	1.64	0.41
1:A:144:LEU:HB2	1:A:146:ASN:OD1	2.21	0.41
1:G:30:GLN:NE2	1:G:198:PRO:HG3	2.35	0.41
1:H:78:PRO:C	1:H:80:SER:N	2.78	0.41
1:I:103:LEU:HD23	1:I:103:LEU:N	2.35	0.41
1:L:121:ILE:CG1	1:L:122:SER:N	2.82	0.41
1:N:48:HIS:ND1	1:N:49:PRO:N	2.69	0.41
1:O:191:CYS:SG	1:O:192:ASN:N	2.93	0.41
1:A:181:PHE:HZ	1:A:199:LEU:HD23	1.85	0.41
1:B:177:HIS:CB	1:B:180:MET:HE3	2.51	0.41
1:C:93:GLU:O	1:C:94:TYR:C	2.62	0.41
1:J:177:HIS:CB	1:J:180:MET:HE3	2.50	0.41
1:K:93:GLU:O	1:K:94:TYR:C	2.60	0.41
1:O:231:LEU:C	1:O:233:LYS:H	2.29	0.41
1:B:29:TRP:CE3	1:B:121:ILE:HB	2.56	0.41
1:B:78:PRO:C	1:B:80:SER:N	2.78	0.41
1:D:123:ILE:HA	1:D:209:LEU:HB3	2.00	0.41
1:E:54:SER:OG	1:E:55:ALA:N	2.53	0.41
1:F:103:LEU:HB3	1:F:229:THR:HG21	2.02	0.41
1:G:139:SER:HA	1:G:156:GLN:O	2.21	0.41
1:G:177:HIS:CB	1:G:180:MET:HE3	2.49	0.41
1:G:208:TYR:CZ	1:K:125:SER:OG	2.64	0.41
1:J:38:GLU:HG2	1:J:40:LEU:H	1.85	0.41
1:O:32:ALA:C	1:O:33:LEU:HD12	2.45	0.41
1:O:103:LEU:HD23	1:O:103:LEU:H	1.84	0.41
1:O:177:HIS:HB3	1:O:180:MET:CE	2.50	0.41
1:A:139:SER:HA	1:A:156:GLN:O	2.21	0.41
1:B:144:LEU:HB2	1:B:146:ASN:OD1	2.21	0.41
1:B:215:PHE:HA	3:B:702:PBZ:C2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:SER:OG	1:C:55:ALA:N	2.53	0.41
1:D:35:MET:HB3	1:D:36:GLU:H	1.51	0.41
1:E:23:SER:HA	1:E:24:PRO:HD3	1.95	0.41
1:H:48:HIS:ND1	1:H:49:PRO:HD2	2.35	0.41
1:I:123:ILE:HA	1:I:209:LEU:HB3	2.02	0.41
1:J:53:LEU:HD12	1:J:53:LEU:HA	1.77	0.41
1:L:69:GLY:N	1:L:118:ILE:HG12	2.36	0.41
1:L:177:HIS:N	1:L:180:MET:HE3	2.35	0.41
1:O:56:ALA:C	1:O:58:CYS:H	2.28	0.41
1:A:23:SER:HB3	1:A:26:SER:HB3	2.03	0.41
1:B:189:ASP:CG	1:B:190:SER:N	2.79	0.41
1:C:40:LEU:C	1:C:40:LEU:CD1	2.93	0.41
1:D:78:PRO:C	1:D:80:SER:N	2.78	0.41
1:E:177:HIS:CB	1:E:180:MET:HE3	2.47	0.41
1:M:38:GLU:HG2	1:M:40:LEU:H	1.84	0.41
1:O:144:LEU:HB2	1:O:146:ASN:OD1	2.21	0.41
1:O:177:HIS:N	1:O:180:MET:HE3	2.34	0.41
1:P:53:LEU:HD12	1:P:53:LEU:HA	1.79	0.41
1:P:123:ILE:HA	1:P:209:LEU:HB3	2.02	0.41
1:A:189:ASP:CG	1:A:190:SER:N	2.79	0.41
1:E:186(A):GLN:HG2	1:F:57:HIS:CD2	2.55	0.41
1:H:48:HIS:CG	1:H:49:PRO:CD	3.03	0.41
1:J:56:ALA:C	1:J:58:CYS:H	2.29	0.41
1:J:96:ARG:HH12	1:O:233:LYS:NZ	2.19	0.41
1:J:200:ILE:HG23	1:J:208:TYR:O	2.21	0.41
1:L:175:LEU:HD23	1:L:175:LEU:HA	1.68	0.41
1:N:189:ASP:CG	1:N:190:SER:N	2.79	0.41
1:D:33:LEU:O	1:D:40:LEU:HD22	2.20	0.41
1:D:189:ASP:CG	1:D:190:SER:N	2.79	0.41
1:D:200:ILE:HA	1:D:208:TYR:O	2.21	0.41
1:F:50:GLN:HG3	1:F:111:SER:CA	2.49	0.41
1:H:56:ALA:C	1:H:58:CYS:H	2.28	0.41
1:I:30:GLN:NE2	1:I:198:PRO:HG3	2.36	0.41
1:I:123:ILE:HD13	1:I:238:ILE:HD13	2.03	0.41
1:K:121:ILE:CG1	1:K:122:SER:N	2.83	0.41
3:L:712:PBZ:N1	4:L:732:HOH:O	2.37	0.41
1:N:200:ILE:HG23	1:N:208:TYR:O	2.20	0.41
1:O:177:HIS:CE1	1:O:178:PRO:HD2	2.55	0.41
1:P:48:HIS:ND1	1:P:49:PRO:CD	2.84	0.41
1:A:50:GLN:HG3	1:A:111:SER:CA	2.50	0.41
1:A:177:HIS:CB	1:A:180:MET:HE3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:HA	1:B:67:LEU:HD23	1.87	0.41
1:C:137:LEU:HG	1:C:138:VAL:N	2.36	0.41
1:D:190:SER:CB	3:D:704:PBZ:HN22	2.26	0.41
1:F:29:TRP:CE3	1:F:121:ILE:HB	2.56	0.41
1:H:123:ILE:HD13	1:H:238:ILE:HD13	2.02	0.41
1:J:60:GLN:HB2	1:J:63:TYR:CE2	2.56	0.41
1:J:78:PRO:C	1:J:80:SER:N	2.79	0.41
1:J:128:CYS:HB3	1:J:129:PRO:CD	2.51	0.41
1:J:177:HIS:N	1:J:180:MET:HE3	2.36	0.41
1:K:22:CYS:O	1:K:71:HIS:HE1	2.04	0.41
1:L:123:ILE:HD13	1:L:238:ILE:HD13	2.03	0.41
1:M:175:LEU:HA	1:M:175:LEU:HD23	1.66	0.41
1:N:40:LEU:C	1:N:40:LEU:CD1	2.94	0.41
1:O:50:GLN:HG3	1:O:111:SER:CA	2.51	0.41
1:P:123:ILE:HD13	1:P:238:ILE:HD13	2.03	0.41
1:C:146:ASN:OD1	1:C:150:ARG:CB	2.68	0.41
1:E:78:PRO:C	1:E:80:SER:N	2.78	0.41
1:F:23:SER:O	1:F:24:PRO:C	2.64	0.41
1:F:93:GLU:O	1:F:94:TYR:C	2.61	0.41
1:I:48:HIS:CE1	1:I:49:PRO:HD2	2.56	0.41
1:L:48:HIS:ND1	1:L:49:PRO:CD	2.84	0.41
1:L:182:CYS:HB3	1:L:225:PRO:HB2	2.03	0.41
1:N:23:SER:O	1:N:24:PRO:C	2.64	0.41
1:N:181:PHE:HZ	1:N:199:LEU:HD23	1.86	0.41
1:O:177:HIS:CD2	1:O:179:SER:H	2.39	0.41
1:A:176:TYR:HE1	1:G:166:GLU:OE2	2.03	0.40
1:C:177:HIS:CB	1:C:180:MET:HE3	2.51	0.40
1:D:69:GLY:N	1:D:118:ILE:HG12	2.37	0.40
1:H:103:LEU:HD23	1:H:103:LEU:N	2.34	0.40
1:J:180:MET:HB2	1:J:227:VAL:CG1	2.51	0.40
1:K:128:CYS:O	1:K:129:PRO:C	2.64	0.40
1:N:97:PRO:O	1:N:98:LEU:C	2.64	0.40
1:O:35:MET:HG2	1:O:41:PHE:CD1	2.56	0.40
1:P:29:TRP:CE3	1:P:121:ILE:HB	2.56	0.40
1:B:139:SER:HA	1:B:156:GLN:O	2.21	0.40
1:C:121:ILE:CG1	1:C:122:SER:N	2.85	0.40
1:D:29:TRP:CE3	1:D:121:ILE:HB	2.57	0.40
1:D:91:HIS:ND1	1:D:92:PRO:HD2	2.36	0.40
1:D:173:ASP:C	1:D:173:ASP:OD1	2.64	0.40
1:E:91:HIS:O	1:E:92:PRO:C	2.64	0.40
1:H:200:ILE:HG23	1:H:208:TYR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:165:GLU:HB3	1:M:165:GLU:HB3	2.02	0.40
1:M:50:GLN:HG3	1:M:111:SER:CA	2.52	0.40
1:M:177:HIS:CE1	1:M:178:PRO:HD2	2.57	0.40
1:A:94:TYR:HA	1:A:101:ASN:HB2	2.04	0.40
1:A:121:ILE:CG1	1:A:122:SER:N	2.84	0.40
1:C:177:HIS:HB3	1:C:180:MET:CE	2.51	0.40
1:F:67:LEU:HA	1:F:67:LEU:HD23	1.89	0.40
1:F:200:ILE:HG23	1:F:208:TYR:O	2.21	0.40
1:G:53:LEU:HA	1:G:53:LEU:HD12	1.77	0.40
1:H:17:ILE:HG13	1:H:220:CYS:HB3	2.03	0.40
1:H:177:HIS:HB3	1:H:180:MET:CE	2.51	0.40
1:I:51:TRP:CZ2	1:I:107:LYS:HD2	2.57	0.40
1:L:103:LEU:HB3	1:L:229:THR:HG21	2.04	0.40
1:P:200:ILE:HA	1:P:208:TYR:O	2.21	0.40
1:P:231:LEU:O	1:P:233:LYS:N	2.55	0.40
1:A:29:TRP:CE3	1:A:121:ILE:HB	2.56	0.40
1:C:33:LEU:O	1:C:40:LEU:HD22	2.22	0.40
1:C:48:HIS:ND1	1:C:49:PRO:CD	2.83	0.40
1:E:91:HIS:HA	1:E:92:PRO:HD3	2.00	0.40
1:F:163:VAL:HG12	1:F:164:SER:N	2.36	0.40
1:G:182:CYS:HB3	1:G:225:PRO:HB2	2.03	0.40
1:L:146:ASN:OD1	1:L:150:ARG:HB2	2.21	0.40
1:M:48:HIS:ND1	1:M:49:PRO:N	2.69	0.40
1:M:103:LEU:HB3	1:M:229:THR:HG21	2.03	0.40
1:M:121:ILE:CG1	1:M:122:SER:N	2.84	0.40
1:N:143:LEU:HB2	1:N:191:CYS:SG	2.62	0.40
1:P:94:TYR:HA	1:P:101:ASN:HB2	2.03	0.40
1:C:35:MET:HG2	1:C:41:PHE:CD1	2.56	0.40
1:E:48:HIS:ND1	1:E:49:PRO:N	2.70	0.40
1:F:40:LEU:C	1:F:40:LEU:CD1	2.94	0.40
1:G:29:TRP:CE3	1:G:121:ILE:HB	2.57	0.40
1:H:22:CYS:SG	1:H:156:GLN:C	3.05	0.40
1:H:33:LEU:O	1:H:40:LEU:HD22	2.21	0.40
1:H:58:CYS:O	1:H:60:GLN:HG2	2.22	0.40
1:I:231:LEU:O	1:I:233:LYS:N	2.54	0.40
1:J:94:TYR:HA	1:J:101:ASN:HB2	2.03	0.40
1:J:243:GLN:HB3	1:J:244:ALA:H	1.63	0.40
1:L:78:PRO:C	1:L:80:SER:N	2.79	0.40
1:L:139:SER:HA	1:L:156:GLN:O	2.21	0.40
1:N:29:TRP:CE3	1:N:121:ILE:HB	2.56	0.40
1:N:32:ALA:C	1:N:33:LEU:HD12	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:78:PRO:C	1:N:80:SER:N	2.79	0.40
1:N:111:SER:N	4:N:733:HOH:O	2.49	0.40
1:P:144:LEU:HB2	1:P:146:ASN:OD1	2.21	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:ARG:NH1	4:F:731:HOH:O[1_565]	1.91	0.29
1:E:84:GLU:OE2	1:G:76:GLN:OE1[2_555]	2.01	0.19
1:B:75:ASP:O	1:C:146:ASN:CB[2_544]	2.02	0.18
1:I:37:ASN:OD1	4:K:720:HOH:O[2_454]	2.09	0.11
1:N:239:GLU:CG	4:L:740:HOH:O[1_545]	2.09	0.11
1:B:75:ASP:C	1:C:146:ASN:ND2[2_544]	2.10	0.10
1:B:75:ASP:O	1:C:146:ASN:ND2[2_544]	2.11	0.09
1:F:116:ASP:OD2	1:H:159:ASN:CG[1_545]	2.17	0.03
1:O:239:GLU:CG	4:C:723:HOH:O[1_455]	2.18	0.02

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	221/223 (99%)	194 (88%)	22 (10%)	5 (2%)	5	25
1	B	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	6	31
1	C	221/223 (99%)	192 (87%)	25 (11%)	4 (2%)	6	31
1	D	221/223 (99%)	196 (89%)	21 (10%)	4 (2%)	6	31
1	E	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	6	31
1	F	221/223 (99%)	198 (90%)	19 (9%)	4 (2%)	6	31
1	G	221/223 (99%)	193 (87%)	24 (11%)	4 (2%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	221/223 (99%)	196 (89%)	19 (9%)	6 (3%)	4	22
1	I	221/223 (99%)	196 (89%)	20 (9%)	5 (2%)	5	25
1	J	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	6	31
1	K	221/223 (99%)	194 (88%)	23 (10%)	4 (2%)	6	31
1	L	221/223 (99%)	194 (88%)	22 (10%)	5 (2%)	5	25
1	M	221/223 (99%)	194 (88%)	23 (10%)	4 (2%)	6	31
1	N	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	6	31
1	O	221/223 (99%)	194 (88%)	22 (10%)	5 (2%)	5	25
1	P	221/223 (99%)	194 (88%)	23 (10%)	4 (2%)	6	31
All	All	3536/3568 (99%)	3115 (88%)	351 (10%)	70 (2%)	6	28

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	B	78	PRO
1	C	78	PRO
1	D	78	PRO
1	E	78	PRO
1	F	78	PRO
1	G	78	PRO
1	H	78	PRO
1	I	78	PRO
1	J	78	PRO
1	K	78	PRO
1	L	78	PRO
1	M	78	PRO
1	N	78	PRO
1	O	78	PRO
1	P	78	PRO
1	A	79	GLY
1	B	79	GLY
1	C	79	GLY
1	D	79	GLY
1	E	79	GLY
1	F	79	GLY
1	G	79	GLY
1	H	79	GLY
1	I	79	GLY

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Mol	Chain	Res	Type
1	J	79	GLY
1	J	243	GLN
1	K	79	GLY
1	L	79	GLY
1	M	79	GLY
1	M	243	GLN
1	N	79	GLY
1	N	243	GLN
1	P	79	GLY
1	A	114	GLU
1	A	243	GLN
1	B	243	GLN
1	C	243	GLN
1	D	114	GLU
1	D	243	GLN
1	E	243	GLN
1	F	243	GLN
1	G	243	GLN
1	H	243	GLN
1	I	243	GLN
1	K	243	GLN
1	L	243	GLN
1	O	79	GLY
1	O	243	GLN
1	P	243	GLN
1	B	114	GLU
1	C	114	GLU
1	E	114	GLU
1	F	114	GLU
1	G	114	GLU
1	H	114	GLU
1	I	114	GLU
1	J	114	GLU
1	K	114	GLU
1	L	114	GLU
1	P	114	GLU
1	A	74	GLU
1	H	74	GLU
1	M	114	GLU
1	N	114	GLU
1	O	74	GLU
1	O	114	GLU

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Mol	Chain	Res	Type
1	H	129	PRO
1	L	158	VAL
1	I	129	PRO

5.3.2 Protein sidechains [i](#)

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	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	B	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	C	189/189 (100%)	175 (93%)	14 (7%)	13	42
1	D	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	E	189/189 (100%)	178 (94%)	11 (6%)	18	51
1	F	189/189 (100%)	178 (94%)	11 (6%)	18	51
1	G	189/189 (100%)	179 (95%)	10 (5%)	20	54
1	H	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	I	189/189 (100%)	179 (95%)	10 (5%)	20	54
1	J	189/189 (100%)	178 (94%)	11 (6%)	18	51
1	K	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	L	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	M	189/189 (100%)	177 (94%)	12 (6%)	16	48
1	N	189/189 (100%)	178 (94%)	11 (6%)	18	51
1	O	189/189 (100%)	178 (94%)	11 (6%)	18	51
1	P	189/189 (100%)	179 (95%)	10 (5%)	20	54
All	All	3024/3024 (100%)	2841 (94%)	183 (6%)	17	49

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	LEU

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Mol	Chain	Res	Type
1	A	88	SER
1	A	122	SER
1	A	127	GLN
1	A	137	LEU
1	A	138	VAL
1	A	150	ARG
1	A	153	THR
1	A	157	CYS
1	A	178	PRO
1	A	180	MET
1	A	190	SER
1	B	87	LEU
1	B	88	SER
1	B	122	SER
1	B	127	GLN
1	B	137	LEU
1	B	138	VAL
1	B	150	ARG
1	B	153	THR
1	B	174	PRO
1	B	178	PRO
1	B	180	MET
1	B	190	SER
1	C	87	LEU
1	C	88	SER
1	C	122	SER
1	C	127	GLN
1	C	136	CYS
1	C	137	LEU
1	C	138	VAL
1	C	150	ARG
1	C	153	THR
1	C	174	PRO
1	C	178	PRO
1	C	180	MET
1	C	190	SER
1	C	201	CYS
1	D	40	LEU
1	D	87	LEU
1	D	88	SER
1	D	122	SER
1	D	127	GLN

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Mol	Chain	Res	Type
1	D	137	LEU
1	D	138	VAL
1	D	150	ARG
1	D	153	THR
1	D	174	PRO
1	D	180	MET
1	D	190	SER
1	E	22	CYS
1	E	87	LEU
1	E	88	SER
1	E	122	SER
1	E	127	GLN
1	E	137	LEU
1	E	138	VAL
1	E	150	ARG
1	E	174	PRO
1	E	180	MET
1	E	190	SER
1	F	22	CYS
1	F	87	LEU
1	F	88	SER
1	F	122	SER
1	F	127	GLN
1	F	137	LEU
1	F	138	VAL
1	F	150	ARG
1	F	178	PRO
1	F	180	MET
1	F	190	SER
1	G	87	LEU
1	G	88	SER
1	G	122	SER
1	G	127	GLN
1	G	137	LEU
1	G	138	VAL
1	G	150	ARG
1	G	174	PRO
1	G	180	MET
1	G	190	SER
1	H	78	PRO
1	H	87	LEU
1	H	88	SER

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Mol	Chain	Res	Type
1	H	122	SER
1	H	127	GLN
1	H	137	LEU
1	H	138	VAL
1	H	150	ARG
1	H	174	PRO
1	H	178	PRO
1	H	180	MET
1	H	190	SER
1	I	87	LEU
1	I	88	SER
1	I	122	SER
1	I	127	GLN
1	I	137	LEU
1	I	138	VAL
1	I	150	ARG
1	I	174	PRO
1	I	180	MET
1	I	190	SER
1	J	87	LEU
1	J	88	SER
1	J	122	SER
1	J	127	GLN
1	J	137	LEU
1	J	138	VAL
1	J	150	ARG
1	J	174	PRO
1	J	178	PRO
1	J	180	MET
1	J	190	SER
1	K	87	LEU
1	K	88	SER
1	K	122	SER
1	K	127	GLN
1	K	137	LEU
1	K	138	VAL
1	K	150	ARG
1	K	153	THR
1	K	174	PRO
1	K	178	PRO
1	K	180	MET
1	K	190	SER

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Mol	Chain	Res	Type
1	L	87	LEU
1	L	88	SER
1	L	122	SER
1	L	127	GLN
1	L	137	LEU
1	L	138	VAL
1	L	150	ARG
1	L	153	THR
1	L	174	PRO
1	L	178	PRO
1	L	180	MET
1	L	190	SER
1	M	40	LEU
1	M	78	PRO
1	M	87	LEU
1	M	88	SER
1	M	122	SER
1	M	127	GLN
1	M	137	LEU
1	M	138	VAL
1	M	150	ARG
1	M	174	PRO
1	M	180	MET
1	M	190	SER
1	N	87	LEU
1	N	88	SER
1	N	122	SER
1	N	127	GLN
1	N	137	LEU
1	N	138	VAL
1	N	150	ARG
1	N	174	PRO
1	N	178	PRO
1	N	180	MET
1	N	190	SER
1	O	87	LEU
1	O	88	SER
1	O	122	SER
1	O	127	GLN
1	O	137	LEU
1	O	138	VAL
1	O	150	ARG

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Mol	Chain	Res	Type
1	O	153	THR
1	O	174	PRO
1	O	180	MET
1	O	190	SER
1	P	87	LEU
1	P	88	SER
1	P	122	SER
1	P	127	GLN
1	P	137	LEU
1	P	138	VAL
1	P	150	ARG
1	P	174	PRO
1	P	180	MET
1	P	190	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	30	GLN
1	A	50	GLN
1	A	61	ASN
1	A	101	ASN
1	A	159	ASN
1	A	177	HIS
1	A	202	ASN
1	A	210	GLN
1	A	221	GLN
1	B	18	ASN
1	B	30	GLN
1	B	50	GLN
1	B	95	ASN
1	B	159	ASN
1	B	177	HIS
1	B	186(A)	GLN
1	B	202	ASN
1	B	210	GLN
1	B	221	GLN
1	C	18	ASN
1	C	30	GLN
1	C	50	GLN
1	C	134	ASN

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Mol	Chain	Res	Type
1	C	177	HIS
1	C	186(A)	GLN
1	C	202	ASN
1	C	210	GLN
1	C	221	GLN
1	C	243	GLN
1	D	18	ASN
1	D	30	GLN
1	D	50	GLN
1	D	177	HIS
1	D	186(A)	GLN
1	D	202	ASN
1	D	210	GLN
1	E	18	ASN
1	E	30	GLN
1	E	76	GLN
1	E	81	GLN
1	E	95	ASN
1	E	101	ASN
1	E	159	ASN
1	E	177	HIS
1	E	202	ASN
1	E	210	GLN
1	E	221	GLN
1	F	18	ASN
1	F	30	GLN
1	F	50	GLN
1	F	95	ASN
1	F	177	HIS
1	F	202	ASN
1	F	210	GLN
1	F	221	GLN
1	F	243	GLN
1	G	18	ASN
1	G	30	GLN
1	G	50	GLN
1	G	156	GLN
1	G	177	HIS
1	G	186(A)	GLN
1	G	202	ASN
1	G	210	GLN
1	G	221	GLN

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Mol	Chain	Res	Type
1	H	18	ASN
1	H	30	GLN
1	H	101	ASN
1	H	159	ASN
1	H	177	HIS
1	H	186(A)	GLN
1	H	202	ASN
1	H	210	GLN
1	H	221	GLN
1	I	18	ASN
1	I	30	GLN
1	I	50	GLN
1	I	95	ASN
1	I	177	HIS
1	I	186(A)	GLN
1	I	210	GLN
1	I	221	GLN
1	J	18	ASN
1	J	30	GLN
1	J	50	GLN
1	J	95	ASN
1	J	134	ASN
1	J	177	HIS
1	J	202	ASN
1	J	210	GLN
1	J	221	GLN
1	J	243	GLN
1	K	18	ASN
1	K	30	GLN
1	K	50	GLN
1	K	71	HIS
1	K	177	HIS
1	K	186(A)	GLN
1	K	202	ASN
1	K	210	GLN
1	K	221	GLN
1	L	18	ASN
1	L	30	GLN
1	L	50	GLN
1	L	177	HIS
1	L	202	ASN
1	L	210	GLN

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Mol	Chain	Res	Type
1	L	243	GLN
1	M	18	ASN
1	M	30	GLN
1	M	50	GLN
1	M	61	ASN
1	M	76	GLN
1	M	95	ASN
1	M	101	ASN
1	M	177	HIS
1	M	202	ASN
1	M	210	GLN
1	M	221	GLN
1	N	18	ASN
1	N	30	GLN
1	N	50	GLN
1	N	177	HIS
1	N	202	ASN
1	N	210	GLN
1	N	221	GLN
1	N	243	GLN
1	O	18	ASN
1	O	30	GLN
1	O	50	GLN
1	O	177	HIS
1	O	202	ASN
1	O	210	GLN
1	O	221	GLN
1	P	18	ASN
1	P	30	GLN
1	P	50	GLN
1	P	177	HIS
1	P	186(A)	GLN
1	P	202	ASN
1	P	210	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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
3	PBZ	G	707	-	10,10,10	2.76	4 (40%)	9,13,13	1.76	3 (33%)
3	PBZ	C	703	-	10,10,10	2.15	4 (40%)	9,13,13	1.81	4 (44%)
3	PBZ	I	709	-	10,10,10	3.66	7 (70%)	9,13,13	0.85	0
3	PBZ	J	710	-	10,10,10	1.96	3 (30%)	9,13,13	1.12	1 (11%)
3	PBZ	K	711	-	10,10,10	2.09	2 (20%)	9,13,13	1.44	1 (11%)
3	PBZ	H	708	-	10,10,10	3.04	6 (60%)	9,13,13	1.43	0
3	PBZ	B	702	-	10,10,10	3.14	4 (40%)	9,13,13	1.44	1 (11%)
3	PBZ	D	704	-	10,10,10	2.34	3 (30%)	9,13,13	1.36	1 (11%)
3	PBZ	E	705	-	10,10,10	3.41	6 (60%)	9,13,13	1.40	1 (11%)
3	PBZ	L	712	-	10,10,10	3.73	9 (90%)	9,13,13	0.82	0
3	PBZ	P	716	-	10,10,10	3.71	8 (80%)	9,13,13	1.12	1 (11%)
3	PBZ	O	715	-	10,10,10	2.50	5 (50%)	9,13,13	2.11	5 (55%)
3	PBZ	A	701	-	10,10,10	4.46	7 (70%)	9,13,13	2.72	5 (55%)
3	PBZ	N	714	-	10,10,10	3.55	5 (50%)	9,13,13	2.04	3 (33%)
3	PBZ	F	706	-	10,10,10	1.70	2 (20%)	9,13,13	1.89	3 (33%)
3	PBZ	M	713	-	10,10,10	1.72	2 (20%)	9,13,13	1.88	3 (33%)

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
3	PBZ	G	707	-	-	2/4/4/4	0/1/1/1
3	PBZ	C	703	-	-	0/4/4/4	0/1/1/1
3	PBZ	I	709	-	-	2/4/4/4	0/1/1/1
3	PBZ	J	710	-	-	1/4/4/4	0/1/1/1
3	PBZ	K	711	-	-	2/4/4/4	0/1/1/1
3	PBZ	H	708	-	-	2/4/4/4	0/1/1/1
3	PBZ	B	702	-	-	2/4/4/4	0/1/1/1
3	PBZ	D	704	-	-	3/4/4/4	0/1/1/1
3	PBZ	E	705	-	-	0/4/4/4	0/1/1/1
3	PBZ	L	712	-	-	4/4/4/4	0/1/1/1
3	PBZ	P	716	-	-	2/4/4/4	0/1/1/1
3	PBZ	O	715	-	-	4/4/4/4	0/1/1/1
3	PBZ	A	701	-	-	3/4/4/4	0/1/1/1
3	PBZ	N	714	-	-	0/4/4/4	0/1/1/1
3	PBZ	F	706	-	-	4/4/4/4	0/1/1/1
3	PBZ	M	713	-	-	0/4/4/4	0/1/1/1

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	PBZ	C4-C7	8.97	1.64	1.47
3	A	701	PBZ	C5-C4	7.74	1.51	1.39
3	B	702	PBZ	C5-C4	7.04	1.50	1.39
3	L	712	PBZ	C4-C7	6.67	1.59	1.47
3	E	705	PBZ	C4-C7	6.48	1.59	1.47
3	P	716	PBZ	C5-C4	6.35	1.49	1.39
3	N	714	PBZ	C6-C5	6.30	1.49	1.38
3	G	707	PBZ	C4-C7	6.12	1.58	1.47
3	P	716	PBZ	C4-C7	5.94	1.58	1.47
3	N	714	PBZ	C3-C4	5.92	1.48	1.39
3	H	708	PBZ	C2-C1	5.65	1.51	1.40
3	E	705	PBZ	C5-C4	5.63	1.48	1.39
3	I	709	PBZ	C3-C2	5.21	1.47	1.38
3	I	709	PBZ	C6-C5	5.17	1.47	1.38
3	L	712	PBZ	C5-C4	5.14	1.47	1.39
3	I	709	PBZ	C5-C4	5.00	1.47	1.39
3	P	716	PBZ	C3-C4	4.97	1.46	1.39
3	O	715	PBZ	C4-C7	4.91	1.56	1.47
3	N	714	PBZ	C6-C1	4.87	1.50	1.40
3	D	704	PBZ	C4-C7	4.54	1.55	1.47
3	I	709	PBZ	C2-C1	4.48	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	PBZ	C4-C7	4.42	1.55	1.47
3	J	710	PBZ	C3-C2	4.36	1.45	1.38
3	K	711	PBZ	C3-C2	4.14	1.45	1.38
3	D	704	PBZ	C6-C5	4.13	1.45	1.38
3	H	708	PBZ	C5-C4	3.95	1.45	1.39
3	H	708	PBZ	C7-N2	-3.86	1.23	1.33
3	A	701	PBZ	C6-C5	3.84	1.45	1.38
3	N	714	PBZ	C3-C2	3.83	1.45	1.38
3	E	705	PBZ	C1-N1	3.80	1.51	1.38
3	K	711	PBZ	C5-C4	-3.74	1.33	1.39
3	L	712	PBZ	C6-C1	3.72	1.47	1.40
3	P	716	PBZ	C3-C2	3.64	1.44	1.38
3	I	709	PBZ	C4-C7	3.63	1.54	1.47
3	F	706	PBZ	C6-C1	-3.61	1.32	1.40
3	O	715	PBZ	C6-C1	-3.55	1.32	1.40
3	O	715	PBZ	C3-C4	-3.52	1.34	1.39
3	A	701	PBZ	C7-N3	3.49	1.42	1.27
3	M	713	PBZ	C6-C1	3.46	1.47	1.40
3	L	712	PBZ	C7-N3	3.38	1.41	1.27
3	E	705	PBZ	C7-N3	3.37	1.41	1.27
3	G	707	PBZ	C2-C1	3.36	1.47	1.40
3	L	712	PBZ	C1-N1	3.28	1.49	1.38
3	C	703	PBZ	C3-C2	3.27	1.44	1.38
3	C	703	PBZ	C3-C4	3.27	1.44	1.39
3	A	701	PBZ	C2-C1	-3.22	1.33	1.40
3	H	708	PBZ	C6-C5	3.20	1.44	1.38
3	C	703	PBZ	C6-C5	3.18	1.43	1.38
3	B	702	PBZ	C3-C2	3.16	1.43	1.38
3	D	704	PBZ	C2-C1	-3.15	1.33	1.40
3	E	705	PBZ	C2-C1	3.13	1.46	1.40
3	F	706	PBZ	C3-C4	-2.98	1.34	1.39
3	I	709	PBZ	C6-C1	2.87	1.46	1.40
3	A	701	PBZ	C7-N2	2.86	1.41	1.33
3	L	712	PBZ	C6-C5	2.86	1.43	1.38
3	M	713	PBZ	C3-C4	2.84	1.43	1.39
3	G	707	PBZ	C7-N2	2.83	1.41	1.33
3	I	709	PBZ	C3-C4	2.82	1.43	1.39
3	L	712	PBZ	C7-N2	2.82	1.41	1.33
3	P	716	PBZ	C7-N3	2.80	1.39	1.27
3	L	712	PBZ	C2-C1	2.75	1.45	1.40
3	C	703	PBZ	C5-C4	-2.72	1.35	1.39
3	H	708	PBZ	C4-C7	2.72	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	707	PBZ	C5-C4	2.68	1.43	1.39
3	A	701	PBZ	C6-C1	2.65	1.45	1.40
3	H	708	PBZ	C1-N1	2.63	1.47	1.38
3	L	712	PBZ	C3-C4	2.54	1.43	1.39
3	O	715	PBZ	C3-C2	2.54	1.42	1.38
3	P	716	PBZ	C2-C1	2.45	1.45	1.40
3	N	714	PBZ	C4-C7	2.42	1.51	1.47
3	P	716	PBZ	C6-C5	2.29	1.42	1.38
3	J	710	PBZ	C5-C4	2.20	1.42	1.39
3	O	715	PBZ	C5-C4	2.18	1.42	1.39
3	B	702	PBZ	C6-C5	2.15	1.42	1.38
3	P	716	PBZ	C6-C1	2.09	1.44	1.40
3	E	705	PBZ	C3-C2	2.05	1.42	1.38
3	J	710	PBZ	C6-C1	-2.03	1.35	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PBZ	C2-C1-N1	-4.85	111.97	120.90
3	A	701	PBZ	C5-C6-C1	-4.36	115.34	120.66
3	F	706	PBZ	C2-C3-C4	-3.88	116.66	120.80
3	N	714	PBZ	C6-C5-C4	-3.73	116.82	120.80
3	O	715	PBZ	C6-C5-C4	3.66	124.71	120.80
3	M	713	PBZ	C6-C5-C4	-3.45	117.11	120.80
3	N	714	PBZ	C2-C3-C4	3.20	124.22	120.80
3	G	707	PBZ	C4-C7-N2	2.96	122.50	118.01
3	B	702	PBZ	C4-C7-N2	2.95	122.50	118.01
3	C	703	PBZ	C3-C2-C1	-2.91	117.10	120.66
3	G	707	PBZ	C6-C1-N1	-2.87	115.61	120.90
3	A	701	PBZ	C6-C1-N1	2.84	126.14	120.90
3	N	714	PBZ	C5-C6-C1	2.80	124.08	120.66
3	M	713	PBZ	C3-C2-C1	-2.75	117.30	120.66
3	O	715	PBZ	C2-C3-C4	-2.68	117.93	120.80
3	O	715	PBZ	C4-C7-N2	2.54	121.86	118.01
3	C	703	PBZ	C6-C5-C4	-2.50	118.12	120.80
3	A	701	PBZ	C6-C1-C2	2.48	121.88	118.16
3	J	710	PBZ	C2-C3-C4	-2.47	118.16	120.80
3	O	715	PBZ	C5-C6-C1	-2.47	117.65	120.66
3	K	711	PBZ	C5-C6-C1	2.42	123.62	120.66
3	A	701	PBZ	C3-C2-C1	2.34	123.53	120.66
3	M	713	PBZ	C5-C4-C3	2.28	121.47	118.57
3	F	706	PBZ	C5-C6-C1	-2.26	117.91	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	704	PBZ	C2-C1-N1	-2.22	116.81	120.90
3	O	715	PBZ	C3-C2-C1	2.21	123.37	120.66
3	C	703	PBZ	C5-C6-C1	2.21	123.36	120.66
3	E	705	PBZ	C6-C5-C4	2.20	123.15	120.80
3	P	716	PBZ	C6-C1-C2	2.16	121.41	118.16
3	F	706	PBZ	C3-C2-C1	2.08	123.20	120.66
3	G	707	PBZ	C2-C1-N1	2.04	124.66	120.90
3	C	703	PBZ	C2-C3-C4	2.02	122.96	120.80

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	704	PBZ	C3-C4-C7-N2
3	D	704	PBZ	C5-C4-C7-N2
3	H	708	PBZ	C3-C4-C7-N2
3	H	708	PBZ	C5-C4-C7-N2
3	K	711	PBZ	C3-C4-C7-N2
3	K	711	PBZ	C5-C4-C7-N2
3	O	715	PBZ	C3-C4-C7-N2
3	O	715	PBZ	C5-C4-C7-N2
3	P	716	PBZ	C3-C4-C7-N2
3	P	716	PBZ	C5-C4-C7-N2
3	B	702	PBZ	C5-C4-C7-N3
3	G	707	PBZ	C5-C4-C7-N2
3	I	709	PBZ	C3-C4-C7-N2
3	I	709	PBZ	C5-C4-C7-N3
3	J	710	PBZ	C3-C4-C7-N2
3	O	715	PBZ	C3-C4-C7-N3
3	O	715	PBZ	C5-C4-C7-N3
3	A	701	PBZ	C3-C4-C7-N2
3	A	701	PBZ	C5-C4-C7-N2
3	F	706	PBZ	C3-C4-C7-N2
3	F	706	PBZ	C5-C4-C7-N2
3	L	712	PBZ	C3-C4-C7-N2
3	L	712	PBZ	C5-C4-C7-N2
3	A	701	PBZ	C3-C4-C7-N3
3	B	702	PBZ	C3-C4-C7-N3
3	D	704	PBZ	C3-C4-C7-N3
3	F	706	PBZ	C3-C4-C7-N3
3	F	706	PBZ	C5-C4-C7-N3
3	G	707	PBZ	C3-C4-C7-N3

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Mol	Chain	Res	Type	Atoms
3	L	712	PBZ	C3-C4-C7-N3
3	L	712	PBZ	C5-C4-C7-N3

There are no ring outliers.

14 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	707	PBZ	2	0
3	I	709	PBZ	2	0
3	J	710	PBZ	2	0
3	H	708	PBZ	5	0
3	B	702	PBZ	2	0
3	D	704	PBZ	7	0
3	E	705	PBZ	2	0
3	L	712	PBZ	1	0
3	P	716	PBZ	6	0
3	O	715	PBZ	8	0
3	A	701	PBZ	2	0
3	N	714	PBZ	2	0
3	F	706	PBZ	1	0
3	M	713	PBZ	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	220/223 (98%)	0.38	10 (4%) 38 20	9, 30, 54, 68	28 (12%)
1	B	222/223 (99%)	0.29	5 (2%) 61 38	7, 28, 51, 65	20 (9%)
1	C	223/223 (100%)	0.31	7 (3%) 51 30	7, 28, 54, 66	18 (8%)
1	D	222/223 (99%)	0.32	9 (4%) 41 23	6, 28, 53, 67	22 (9%)
1	E	223/223 (100%)	0.27	8 (3%) 46 26	7, 26, 52, 65	24 (10%)
1	F	223/223 (100%)	0.30	10 (4%) 38 20	4, 26, 51, 64	17 (7%)
1	G	223/223 (100%)	0.47	10 (4%) 38 20	5, 29, 54, 64	20 (8%)
1	H	223/223 (100%)	0.32	7 (3%) 51 30	9, 27, 53, 68	30 (13%)
1	I	223/223 (100%)	0.44	9 (4%) 42 23	10, 29, 50, 64	30 (13%)
1	J	223/223 (100%)	0.33	4 (1%) 67 44	7, 30, 53, 64	18 (8%)
1	K	222/223 (99%)	0.36	5 (2%) 61 38	5, 28, 54, 63	22 (9%)
1	L	223/223 (100%)	0.26	7 (3%) 51 30	5, 30, 54, 67	20 (8%)
1	M	223/223 (100%)	0.28	10 (4%) 38 20	5, 26, 50, 62	16 (7%)
1	N	223/223 (100%)	0.28	10 (4%) 38 20	4, 27, 54, 68	18 (8%)
1	O	223/223 (100%)	0.28	8 (3%) 46 26	6, 26, 52, 63	19 (8%)
1	P	223/223 (100%)	0.34	7 (3%) 51 30	8, 29, 53, 65	23 (10%)
All	All	3562/3568 (99%)	0.33	126 (3%) 47 27	4, 28, 54, 68	345 (9%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	SER	7.2
1	I	190	SER	7.1
1	M	190	SER	6.7
1	K	190	SER	6.7
1	A	190	SER	6.7

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Mol	Chain	Res	Type	RSRZ
1	P	190	SER	6.4
1	B	150	ARG	6.2
1	L	190	SER	5.9
1	H	190	SER	5.7
1	P	150	ARG	5.6
1	B	45	VAL	5.6
1	D	190	SER	5.4
1	C	190	SER	5.3
1	I	150	ARG	5.2
1	N	190	SER	4.9
1	P	45	VAL	4.9
1	O	190	SER	4.8
1	G	190	SER	4.6
1	F	190	SER	4.5
1	O	45	VAL	4.5
1	H	45	VAL	4.4
1	K	45	VAL	4.4
1	F	150	ARG	4.4
1	I	45	VAL	4.4
1	I	75	ASP	4.3
1	E	75	ASP	4.3
1	D	150	ARG	4.3
1	J	190	SER	4.3
1	C	45	VAL	4.3
1	E	145	ALA	4.3
1	M	36	GLU	4.2
1	I	76	GLN	4.2
1	E	190	SER	4.1
1	M	45	VAL	4.1
1	G	150	ARG	4.1
1	G	45	VAL	4.0
1	I	36	GLU	3.9
1	O	150	ARG	3.8
1	J	45	VAL	3.8
1	F	45	VAL	3.7
1	J	243	GLN	3.6
1	N	45	VAL	3.6
1	E	150	ARG	3.6
1	O	75	ASP	3.5
1	N	75	ASP	3.4
1	C	146	ASN	3.4
1	E	45	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	75	ASP	3.2
1	D	45	VAL	3.2
1	B	147	GLY	3.1
1	N	150	ARG	3.1
1	P	74(A)	ALA	3.0
1	A	45	VAL	3.0
1	A	36	GLU	3.0
1	C	142	GLY	3.0
1	F	243	GLN	3.0
1	H	76	GLN	3.0
1	N	147	GLY	3.0
1	L	45	VAL	3.0
1	F	244	ALA	3.0
1	L	150	ARG	2.9
1	M	78	PRO	2.9
1	F	36	GLU	2.8
1	O	208	TYR	2.7
1	G	110	GLU	2.7
1	I	152	PRO	2.6
1	C	74(A)	ALA	2.6
1	A	150	ARG	2.6
1	L	244	ALA	2.6
1	N	243	GLN	2.5
1	E	37	ASN	2.5
1	G	75	ASP	2.5
1	F	109	ASP	2.5
1	M	75	ASP	2.5
1	N	125	SER	2.5
1	N	36	GLU	2.5
1	C	150	ARG	2.5
1	D	133	GLY	2.5
1	L	133	GLY	2.4
1	L	142	GLY	2.4
1	G	117	THR	2.4
1	L	243	GLN	2.4
1	G	142	GLY	2.3
1	H	150	ARG	2.3
1	M	76	GLN	2.3
1	B	49	PRO	2.3
1	H	80	SER	2.3
1	H	244	ALA	2.3
1	E	76	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	243	GLN	2.3
1	N	116	ASP	2.3
1	D	75	ASP	2.3
1	O	34	VAL	2.3
1	O	78	PRO	2.2
1	A	244	ALA	2.2
1	P	113	SER	2.2
1	A	75	ASP	2.2
1	E	152	PRO	2.2
1	M	79	GLY	2.2
1	D	114	GLU	2.2
1	F	20	GLU	2.2
1	M	116	ASP	2.2
1	D	85	ALA	2.2
1	P	143	LEU	2.2
1	A	74	GLU	2.2
1	I	244	ALA	2.2
1	O	36	GLU	2.2
1	N	23	SER	2.1
1	P	151	MET	2.1
1	G	239	GLU	2.1
1	M	37	ASN	2.1
1	K	76	GLN	2.1
1	C	147	GLY	2.1
1	D	78	PRO	2.1
1	G	36	GLU	2.1
1	G	84	GLU	2.1
1	J	61	ASN	2.1
1	A	111	SER	2.0
1	D	62	SER	2.0
1	I	208	TYR	2.0
1	F	147	GLY	2.0
1	A	115	SER	2.0
1	A	76	GLN	2.0
1	K	38	GLU	2.0
1	K	162	VAL	2.0
1	F	73	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CO	A	1	1/1	0.75	0.10	62,62,62,62	0
3	PBZ	G	707	10/10	0.77	0.22	62,65,66,67	0
3	PBZ	C	703	10/10	0.83	0.15	34,39,41,42	0
3	PBZ	N	714	10/10	0.84	0.15	33,39,41,45	0
3	PBZ	H	708	10/10	0.85	0.14	27,31,34,36	0
3	PBZ	L	712	10/10	0.86	0.13	35,37,42,45	0
3	PBZ	M	713	10/10	0.86	0.13	24,26,28,33	0
3	PBZ	B	702	10/10	0.86	0.17	40,47,50,53	0
3	PBZ	E	705	10/10	0.87	0.14	14,30,31,32	0
3	PBZ	P	716	10/10	0.87	0.11	25,33,34,36	0
3	PBZ	O	715	10/10	0.88	0.15	37,39,46,48	0
3	PBZ	I	709	10/10	0.88	0.15	45,46,48,50	0
3	PBZ	J	710	10/10	0.89	0.14	38,39,42,42	0
3	PBZ	A	701	10/10	0.89	0.13	14,19,26,33	0
3	PBZ	K	711	10/10	0.90	0.12	32,36,39,42	0
3	PBZ	F	706	10/10	0.90	0.12	22,26,28,28	0
3	PBZ	D	704	10/10	0.92	0.11	17,21,22,24	0
2	CO	I	3	1/1	0.95	0.06	63,63,63,63	0
2	CO	E	2	1/1	0.98	0.07	35,35,35,35	0
2	CO	M	4	1/1	0.99	0.06	28,28,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.