



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:42 PM EDT

PDB ID : 3FEQ / pdb_00003feq
Title : Crystal structure of uncharacterized protein eah89906
Authors : Patskovsky, Y.; Bonanno, J.; Romero, R.; Freeman, J.; Lau, C.; Smith, D.; Bain, K.; Wasserman, S.R.; Raushel, F.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-11-30
Resolution : 2.63 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

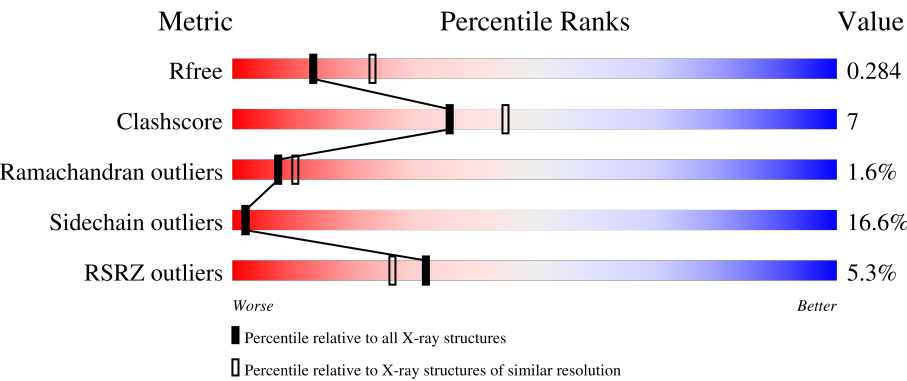
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.63 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	423	3% 70% 22%
1	B	423	3% 69% 22%
1	C	423	4% 70% 22% 5%
1	D	423	6% 70% 21%
1	E	423	3% 73% 19%

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Mol	Chain	Length	Quality of chain
1	F	423	
1	G	423	
1	H	423	
1	I	423	
1	J	423	
1	K	423	
1	L	423	
1	M	423	
1	N	423	
1	O	423	
1	P	423	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 48417 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 PUTATIVE AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	4	0
			3028	1886	547	580	15			
1	B	405	Total	C	N	O	S	0	6	0
			3040	1894	552	579	15			
1	C	406	Total	C	N	O	S	0	2	0
			3025	1883	550	577	15			
1	D	405	Total	C	N	O	S	0	4	0
			3035	1890	553	577	15			
1	E	405	Total	C	N	O	S	0	4	0
			3026	1883	550	578	15			
1	F	405	Total	C	N	O	S	0	2	0
			3016	1878	546	577	15			
1	G	405	Total	C	N	O	S	0	2	0
			3021	1881	549	576	15			
1	H	405	Total	C	N	O	S	0	2	0
			3016	1878	546	577	15			
1	I	405	Total	C	N	O	S	0	1	0
			3013	1876	546	576	15			
1	J	402	Total	C	N	O	S	0	1	0
			2994	1866	543	571	14			
1	K	403	Total	C	N	O	S	0	1	0
			3000	1869	544	572	15			
1	L	404	Total	C	N	O	S	0	1	0
			3005	1870	545	575	15			
1	M	406	Total	C	N	O	S	0	1	0
			3017	1878	547	577	15			
1	N	404	Total	C	N	O	S	0	1	0
			3003	1869	545	575	14			
1	O	401	Total	C	N	O	S	0	1	0
			2983	1857	542	570	14			
1	P	405	Total	C	N	O	S	0	2	0
			3018	1879	547	577	15			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0
2	G	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0
2	I	2	Total 2	Zn 2	0	0
2	J	2	Total 2	Zn 2	0	0
2	K	2	Total 2	Zn 2	0	0
2	L	2	Total 2	Zn 2	0	0
2	M	2	Total 2	Zn 2	0	0
2	N	2	Total 2	Zn 2	0	0
2	O	2	Total 2	Zn 2	0	0
2	P	2	Total 2	Zn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total 24	O 24	0	0
3	B	27	Total 27	O 27	0	0
3	C	13	Total 13	O 13	0	0

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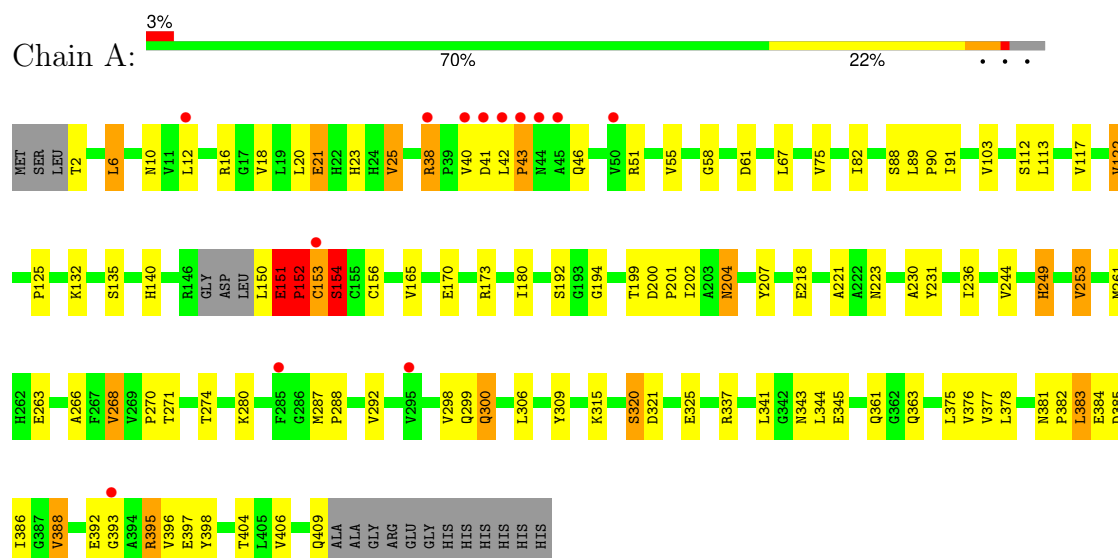
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	20	Total 20	O 20	0	0
3	E	18	Total 18	O 18	0	0
3	F	17	Total 17	O 17	0	0
3	G	16	Total 16	O 16	0	0
3	H	6	Total 6	O 6	0	0
3	O	2	Total 2	O 2	0	0
3	P	2	Total 2	O 2	0	0

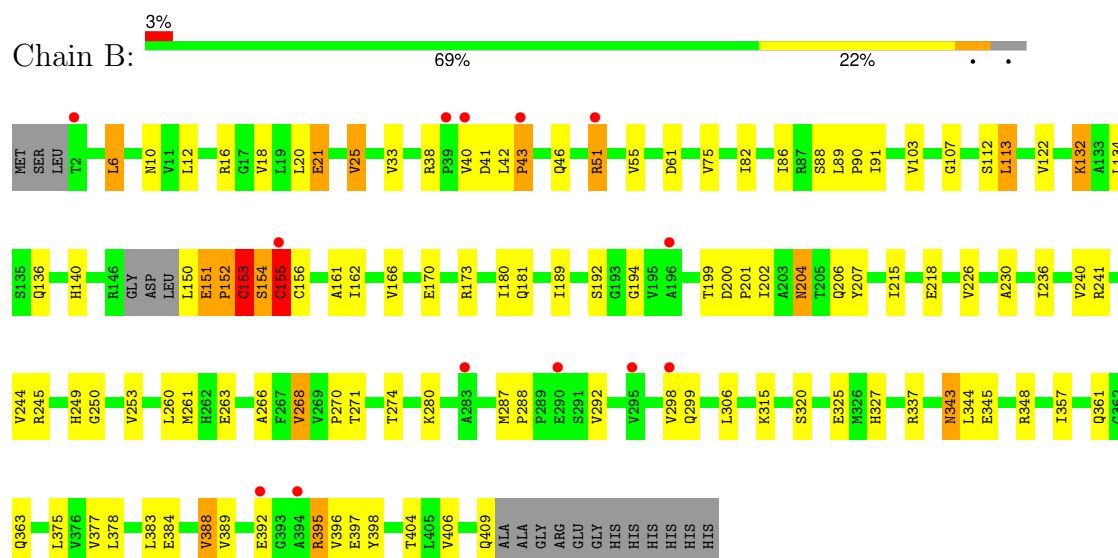
3 Residue-property plots

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

• Molecule 1: PUTATIVE AMIDOHYDROLASE

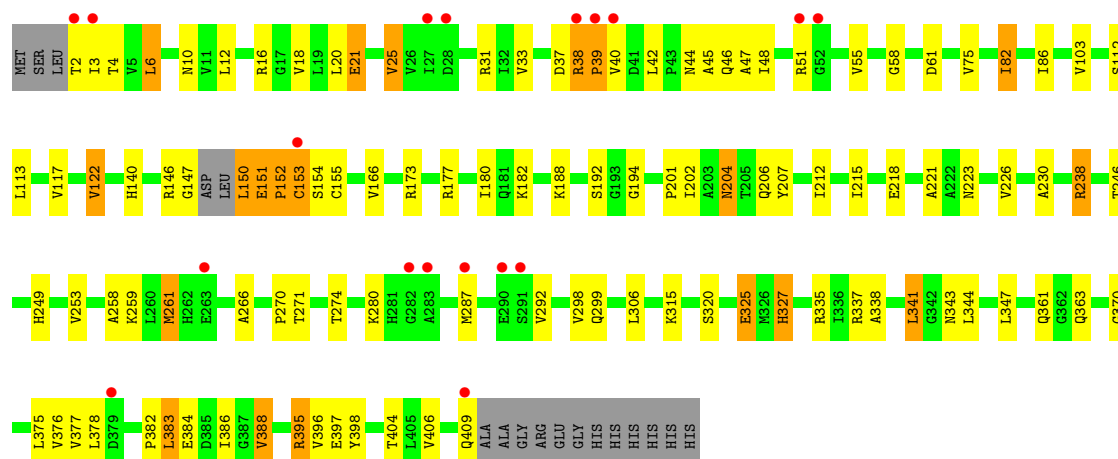


• Molecule 1: PUTATIVE AMIDOHYDROLASE

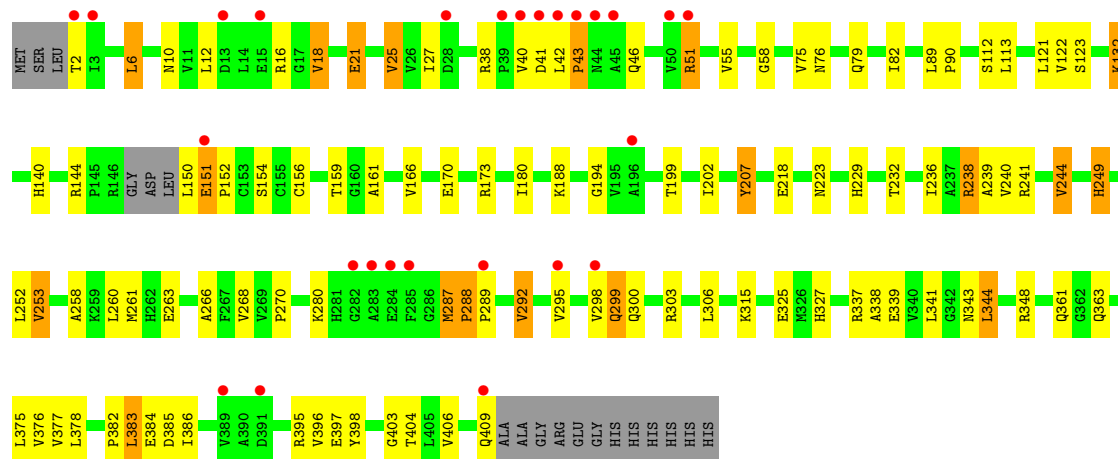


• Molecule 1: PUTATIVE AMIDOHYDROLASE

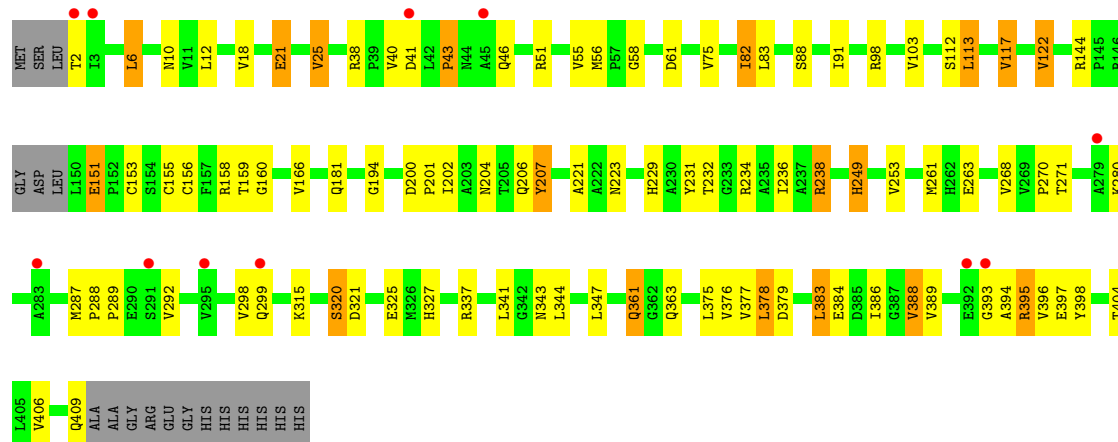
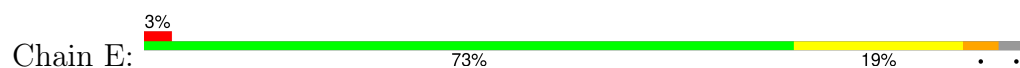




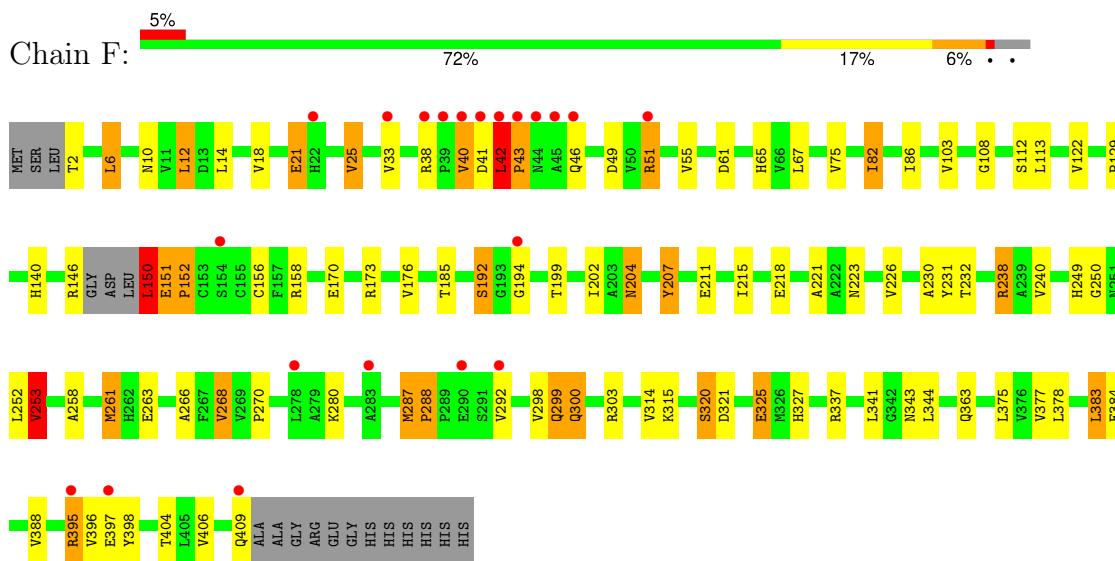
• Molecule 1: PUTATIVE AMIDOHYDROLASE



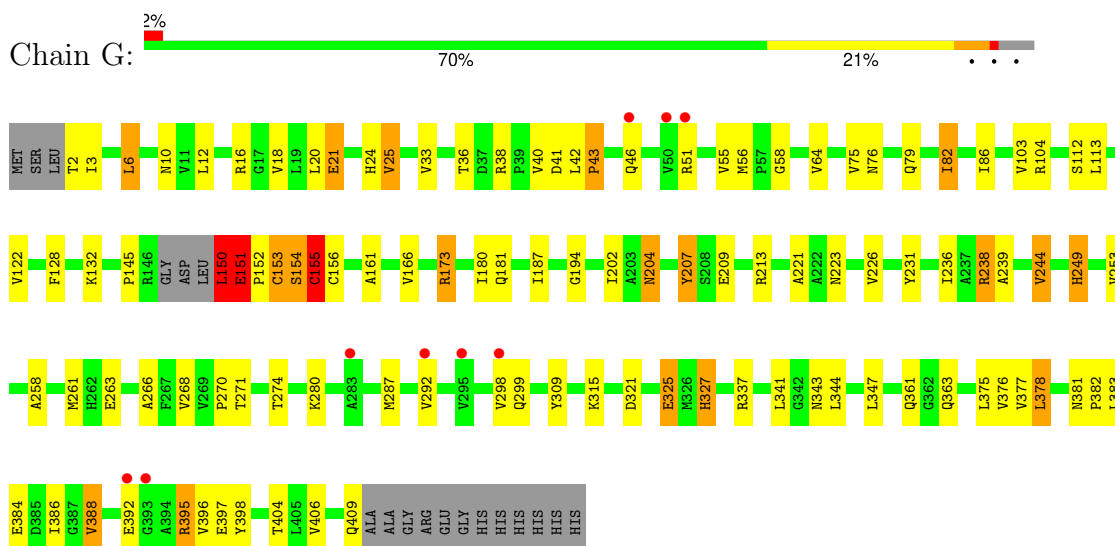
• Molecule 1: PUTATIVE AMIDOHYDROLASE



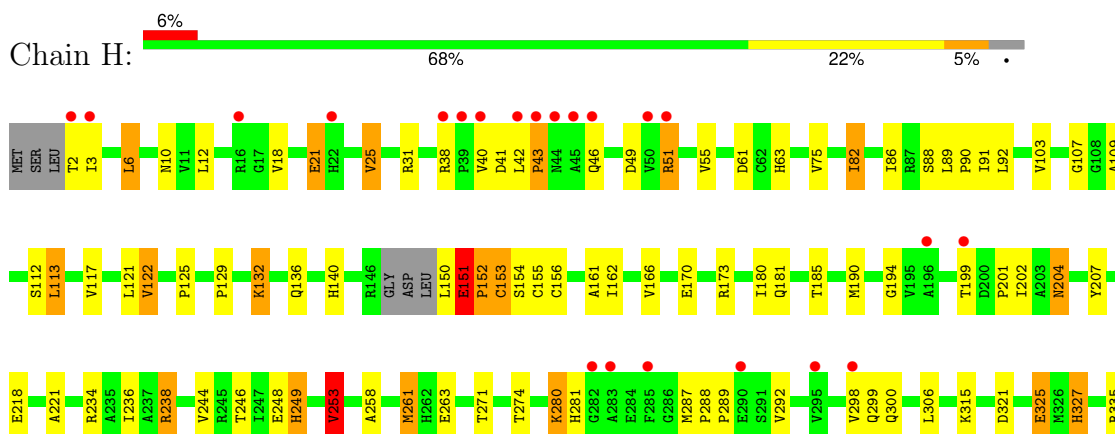
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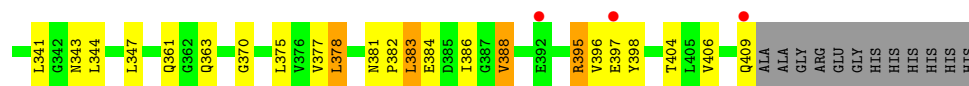


• Molecule 1: PUTATIVE AMIDOHYDROLASE



● Molecule 1: PUTATIVE AMIDOHYDROLASE

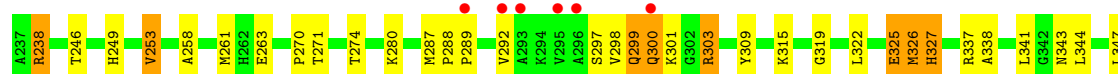
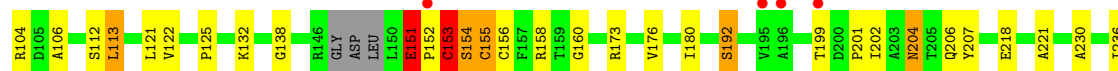
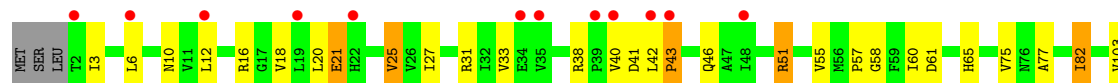




● Molecule 1: PUTATIVE AMIDOHYDROLASE



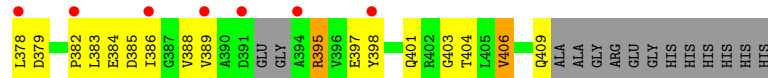
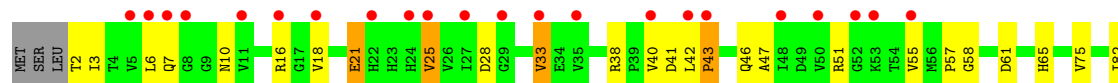
Chain I:



● Molecule 1: PUTATIVE AMIDOHYDROLASE



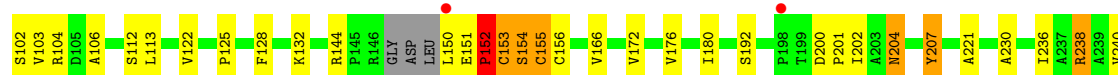
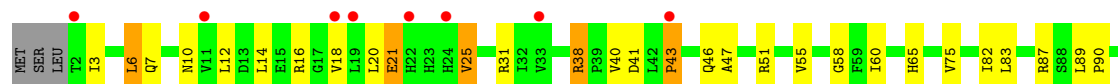
Chain J:

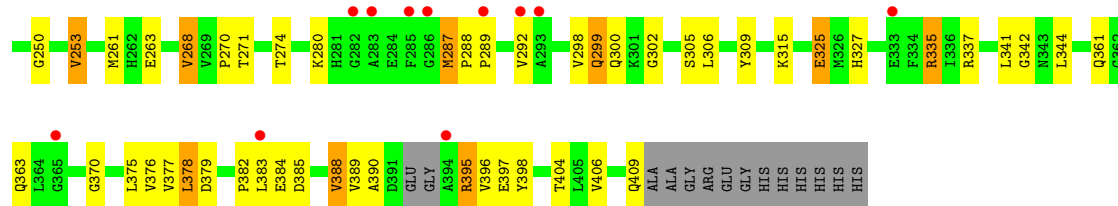


● Molecule 1: PUTATIVE AMIDOHYDROLASE

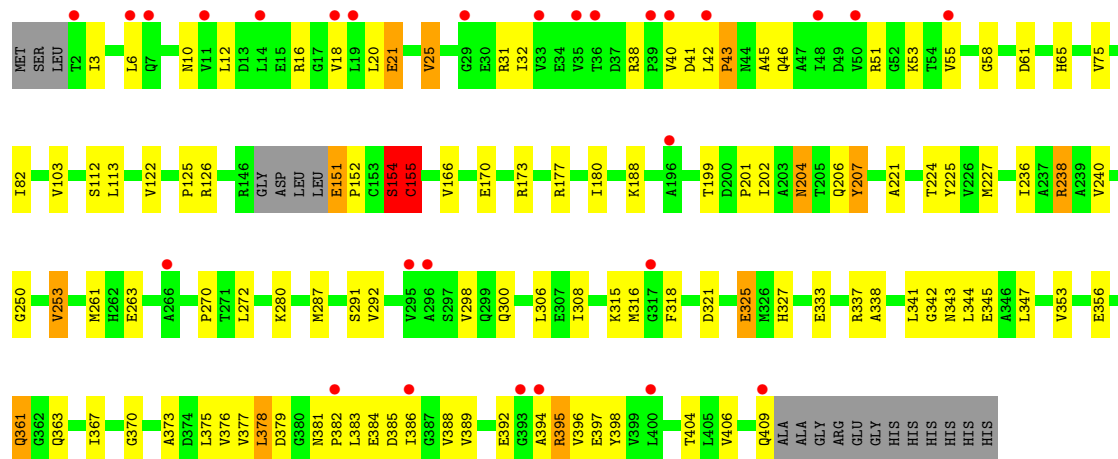


Chain K:

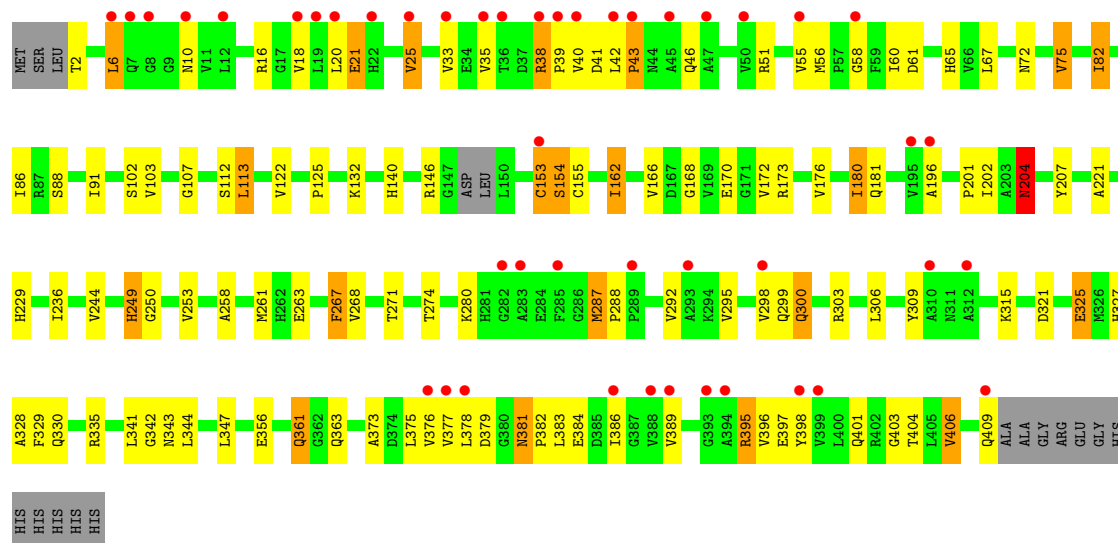




• Molecule 1: PUTATIVE AMIDOHYDROLASE



• Molecule 1: PUTATIVE AMIDOHYDROLASE



• Molecule 1: PUTATIVE AMIDOHYDROLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	113.21Å 108.05Å 171.13Å 81.75° 80.36° 74.40°	Depositor
Resolution (Å)	20.00 – 2.63 20.00 – 2.63	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-2.63) 96.2 (20.00-2.63)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.238 , 0.281 0.242 , 0.284	Depositor DCC
R_{free} test set	6591 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.011 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48417	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/3083	0.86	5/4180 (0.1%)
1	B	0.60	0/3102	0.87	5/4205 (0.1%)
1	C	0.58	0/3074	0.86	3/4167 (0.1%)
1	D	0.61	0/3090	0.87	5/4188 (0.1%)
1	E	0.57	0/3081	0.87	2/4177 (0.0%)
1	F	0.56	0/3065	0.89	7/4156 (0.2%)
1	G	0.54	0/3070	0.88	7/4162 (0.2%)
1	H	0.60	0/3065	0.86	5/4156 (0.1%)
1	I	0.61	0/3059	0.89	5/4148 (0.1%)
1	J	0.56	0/3038	0.86	6/4117 (0.1%)
1	K	0.56	0/3045	0.89	2/4128 (0.0%)
1	L	0.56	0/3051	0.90	6/4137 (0.1%)
1	M	0.56	0/3063	0.89	5/4153 (0.1%)
1	N	0.58	1/3048 (0.0%)	0.86	4/4132 (0.1%)
1	O	0.56	0/3028	0.86	4/4105 (0.1%)
1	P	0.55	0/3067	0.89	5/4159 (0.1%)
All	All	0.57	1/49029 (0.0%)	0.87	76/66470 (0.1%)

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	4
1	B	0	2
1	C	0	3
1	D	0	2
1	E	0	3
1	F	0	2
1	G	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	4
1	I	0	2
1	J	0	3
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	1
1	O	0	3
1	P	0	5
All	All	0	46

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	63	HIS	CA-C	-6.20	1.47	1.53

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	381	ASN	CA-C-N	6.83	126.46	119.56
1	L	381	ASN	C-N-CA	6.83	126.46	119.56
1	H	156	CYS	N-CA-C	6.82	119.53	109.24
1	L	287	MET	CA-C-N	6.61	127.19	120.38
1	L	287	MET	C-N-CA	6.61	127.19	120.38
1	G	151	GLU	CA-C-N	6.44	127.89	119.84
1	G	151	GLU	C-N-CA	6.44	127.89	119.84
1	G	287	MET	CA-C-N	6.36	126.93	120.38
1	G	287	MET	C-N-CA	6.36	126.93	120.38
1	E	287	MET	CA-C-N	6.25	126.82	120.38
1	E	287	MET	C-N-CA	6.25	126.82	120.38
1	F	42	LEU	CA-C-N	-6.25	112.03	119.84
1	F	42	LEU	C-N-CA	-6.25	112.03	119.84
1	J	287	MET	CA-C-N	6.21	126.78	120.38
1	J	287	MET	C-N-CA	6.21	126.78	120.38
1	C	287	MET	CA-C-N	6.20	126.77	120.38
1	C	287	MET	C-N-CA	6.20	126.77	120.38
1	H	287	MET	CA-C-N	6.14	126.71	120.38
1	H	287	MET	C-N-CA	6.14	126.71	120.38
1	L	151	GLU	CA-C-N	6.10	127.46	119.84
1	L	151	GLU	C-N-CA	6.10	127.46	119.84
1	M	204	ASN	N-CA-C	6.06	119.96	110.32
1	K	287	MET	CA-C-N	6.01	126.57	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	287	MET	C-N-CA	6.01	126.57	120.38
1	H	154	SER	N-CA-C	6.01	117.23	107.32
1	O	287	MET	CA-C-N	5.86	126.42	120.38
1	O	287	MET	C-N-CA	5.86	126.42	120.38
1	I	287	MET	CA-C-N	5.85	126.41	120.38
1	I	287	MET	C-N-CA	5.85	126.41	120.38
1	J	151	GLU	N-CA-C	5.78	122.58	109.81
1	D	287	MET	CA-C-N	5.70	126.25	120.38
1	D	287	MET	C-N-CA	5.70	126.25	120.38
1	B	287	MET	CA-C-N	5.68	126.23	120.38
1	B	287	MET	C-N-CA	5.68	126.23	120.38
1	I	359	ASN	N-CA-C	5.65	119.22	111.54
1	F	253	VAL	CB-CA-C	-5.61	103.53	111.28
1	P	288	PRO	CA-C-N	5.59	125.42	119.28
1	P	288	PRO	C-N-CA	5.59	125.42	119.28
1	N	287	MET	CA-C-N	5.56	126.11	120.38
1	N	287	MET	C-N-CA	5.56	126.11	120.38
1	M	287	MET	CA-C-N	5.50	126.05	120.38
1	M	287	MET	C-N-CA	5.50	126.05	120.38
1	F	287	MET	CA-C-N	5.47	126.02	120.38
1	F	287	MET	C-N-CA	5.47	126.02	120.38
1	I	381	ASN	CA-C-N	5.42	125.25	119.28
1	I	381	ASN	C-N-CA	5.42	125.25	119.28
1	P	204	ASN	N-CA-C	5.42	118.89	110.17
1	A	287	MET	CA-C-N	5.42	125.96	120.38
1	A	287	MET	C-N-CA	5.42	125.96	120.38
1	M	381	ASN	CA-C-N	5.39	125.01	119.56
1	M	381	ASN	C-N-CA	5.39	125.01	119.56
1	F	288	PRO	CA-C-N	5.38	125.45	119.32
1	F	288	PRO	C-N-CA	5.38	125.45	119.32
1	G	381	ASN	CA-C-N	5.36	124.97	119.56
1	G	381	ASN	C-N-CA	5.36	124.97	119.56
1	B	288	PRO	CA-C-N	5.34	125.16	119.28
1	B	288	PRO	C-N-CA	5.34	125.16	119.28
1	D	288	PRO	CA-C-N	5.30	125.11	119.28
1	D	288	PRO	C-N-CA	5.30	125.11	119.28
1	J	151	GLU	CA-C-N	5.29	126.45	119.84
1	J	151	GLU	C-N-CA	5.29	126.45	119.84
1	H	253	VAL	CB-CA-C	-5.23	104.41	111.63
1	A	154	SER	N-CA-C	5.22	116.54	107.93
1	B	268	VAL	CB-CA-C	-5.20	102.81	110.82
1	O	288	PRO	CA-C-N	5.19	125.49	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	288	PRO	C-N-CA	5.19	125.49	119.47
1	G	155	CYS	N-CA-C	5.12	118.51	111.54
1	J	253	VAL	CB-CA-C	-5.12	104.22	111.28
1	A	288	PRO	CA-C-N	5.09	124.88	119.28
1	A	288	PRO	C-N-CA	5.09	124.88	119.28
1	N	381	ASN	CA-C-N	5.09	124.88	119.28
1	N	381	ASN	C-N-CA	5.09	124.88	119.28
1	P	287	MET	CA-C-N	5.08	125.61	120.38
1	P	287	MET	C-N-CA	5.08	125.61	120.38
1	C	204	ASN	N-CA-C	5.06	117.98	110.14
1	D	253	VAL	CB-CA-C	-5.03	103.69	111.08

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	GLU	Peptide
1	A	152	PRO	Peptide
1	A	2	THR	Peptide
1	A	38	ARG	Peptide
1	B	155	CYS	Peptide
1	B	38	ARG	Peptide
1	C	152	PRO	Peptide
1	C	153	CYS	Peptide
1	C	2	THR	Peptide
1	D	2	THR	Peptide
1	D	38	ARG	Peptide
1	E	153	CYS	Peptide
1	E	2	THR	Peptide
1	E	38	ARG	Peptide
1	F	150	LEU	Peptide
1	F	2	THR	Peptide
1	G	150	LEU	Peptide
1	G	151	GLU	Peptide
1	G	153	CYS	Peptide
1	G	155	CYS	Peptide
1	G	2	THR	Peptide
1	G	38	ARG	Peptide
1	H	151	GLU	Peptide
1	H	153	CYS	Peptide
1	H	2	THR	Peptide
1	H	38	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	I	151	GLU	Peptide
1	I	38	ARG	Peptide
1	J	151	GLU	Peptide
1	J	2	THR	Peptide
1	J	38	ARG	Peptide
1	K	152	PRO	Peptide
1	K	38	ARG	Peptide
1	L	151	GLU	Peptide
1	L	38	ARG	Peptide
1	M	2	THR	Peptide
1	M	38	ARG	Peptide
1	N	38	ARG	Peptide
1	O	2	THR	Peptide
1	O	361	GLN	Peptide
1	O	38	ARG	Peptide
1	P	150	LEU	Peptide
1	P	151	GLU	Peptide
1	P	152	PRO	Peptide
1	P	2	THR	Peptide
1	P	38	ARG	Peptide

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	3028	0	3044	48	0
1	B	3040	0	3063	47	0
1	C	3025	0	3041	47	1
1	D	3035	0	3059	45	0
1	E	3026	0	3040	43	0
1	F	3016	0	3030	46	0
1	G	3021	0	3038	43	0
1	H	3016	0	3030	53	0
1	I	3013	0	3025	62	1
1	J	2994	0	3009	41	0
1	K	3000	0	3015	43	0
1	L	3005	0	3014	43	0
1	M	3017	0	3028	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	3003	0	3014	56	0
1	O	2983	0	2996	38	0
1	P	3018	0	3031	43	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	24	0	0	0	0
3	B	27	0	0	1	0
3	C	13	0	0	1	0
3	D	20	0	0	1	0
3	E	18	0	0	3	0
3	F	17	0	0	1	0
3	G	16	0	0	1	0
3	H	6	0	0	1	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
All	All	48417	0	48477	704	1

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 7.

All (704) 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:H:263:GLU:OE2	1:M:38:ARG:HD2	1.55	1.07
1:I:221:ALA:O	1:K:204:ASN:HB2	1.60	1.01
1:A:16:ARG:HH12	1:A:20:LEU:HD21	1.27	0.97
1:C:221:ALA:O	1:F:204:ASN:HB2	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ILE:HG23	1:C:45:ALA:HA	1.59	0.85
1:M:153:CYS:O	1:M:154:SER:HB3	1.76	0.84
1:M:377:VAL:HB	1:M:398:TYR:HB2	1.60	0.84
1:A:392:GLU:CG	1:A:393:GLY:H	1.89	0.84
1:J:221:ALA:O	1:L:204:ASN:HB2	1.77	0.84
1:D:16:ARG:HG2	1:D:18:VAL:HG22	1.60	0.84
1:G:377:VAL:HB	1:G:398:TYR:HB2	1.61	0.82
1:L:154:SER:O	1:L:155:CYS:HB2	1.77	0.82
1:C:377:VAL:HB	1:C:398:TYR:HB2	1.59	0.82
1:E:221:ALA:O	1:H:204:ASN:HB2	1.79	0.82
1:I:377:VAL:HB	1:I:398:TYR:HB2	1.62	0.81
1:M:221:ALA:O	1:P:204:ASN:HB2	1.81	0.81
1:K:221:ALA:O	1:N:204:ASN:HB2	1.81	0.80
1:C:147:GLY:HA3	1:C:150:LEU:HB2	1.64	0.80
1:B:16:ARG:HD2	1:N:51:ARG:HG3	1.64	0.79
1:H:150:LEU:O	1:H:151:GLU:HB2	1.81	0.79
1:A:204:ASN:HB2	1:G:221:ALA:O	1.83	0.78
1:M:6:LEU:HB2	1:M:25:VAL:HG13	1.66	0.78
1:J:377:VAL:HB	1:J:398:TYR:HB2	1.68	0.76
1:F:377:VAL:HB	1:F:398:TYR:HB2	1.68	0.76
1:N:146:ARG:CG	1:N:147:GLY:H	2.00	0.75
1:D:16:ARG:HG2	1:D:18:VAL:CG2	2.17	0.75
1:D:207:TYR:O	1:D:238:ARG:NH1	2.21	0.74
1:K:153:CYS:SG	1:K:154:SER:N	2.60	0.74
1:I:207:TYR:O	1:I:238:ARG:NH1	2.21	0.73
1:F:207:TYR:O	1:F:238:ARG:NH1	2.20	0.73
1:A:16:ARG:NH1	1:A:20:LEU:HD21	2.03	0.72
1:A:223:ASN:ND2	1:C:204:ASN:HB3	2.04	0.72
1:A:392:GLU:HG3	1:A:393:GLY:H	1.52	0.72
1:B:153:CYS:O	1:B:154:SER:HB3	1.88	0.71
1:B:377:VAL:HB	1:B:398:TYR:HB2	1.73	0.71
1:N:154:SER:O	1:N:155:CYS:HB3	1.91	0.71
1:H:377:VAL:HB	1:H:398:TYR:HB2	1.73	0.71
1:P:377:VAL:HB	1:P:398:TYR:HB2	1.72	0.71
1:O:16:ARG:HH12	1:O:20:LEU:HD21	1.56	0.70
1:F:221:ALA:O	1:G:204:ASN:HB2	1.91	0.70
1:G:207:TYR:O	1:G:238:ARG:NH1	2.23	0.70
1:B:204:ASN:HB2	1:H:221:ALA:O	1.92	0.69
1:E:377:VAL:HB	1:E:398:TYR:HB2	1.73	0.69
1:I:204:ASN:HB2	1:O:221:ALA:O	1.92	0.69
1:A:377:VAL:HB	1:A:398:TYR:HB2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:6:LEU:HB2	1:J:25:VAL:HG13	1.73	0.69
1:C:4:THR:HG23	1:C:46:GLN:O	1.92	0.69
1:G:150:LEU:O	1:G:151:GLU:HG2	1.91	0.69
1:O:377:VAL:HB	1:O:398:TYR:HB2	1.73	0.69
1:N:377:VAL:HB	1:N:398:TYR:HB2	1.75	0.69
1:C:207:TYR:O	1:C:238:ARG:NH1	2.25	0.68
1:P:236:ILE:HG21	1:P:261:MET:HE2	1.75	0.68
1:F:10:ASN:HD22	1:F:21:GLU:HA	1.58	0.68
1:J:150:LEU:O	1:J:151:GLU:HB2	1.93	0.68
1:N:146:ARG:HG3	1:N:147:GLY:H	1.58	0.68
1:B:245:ARG:NH1	1:B:357:ILE:O	2.25	0.68
1:I:151:GLU:HB3	1:I:152:PRO:HD3	1.75	0.68
1:N:192:SER:HB2	1:N:230:ALA:HA	1.76	0.68
1:O:206:GLN:O	1:O:207:TYR:HB2	1.93	0.68
1:B:41:ASP:O	1:B:43:PRO:HD3	1.95	0.67
1:N:146:ARG:CG	1:N:147:GLY:N	2.56	0.67
1:M:343:ASN:HD22	1:M:386:ILE:HB	1.60	0.67
1:D:150:LEU:C	1:D:151:GLU:HG3	2.18	0.66
1:E:207:TYR:O	1:E:238:ARG:NH1	2.29	0.66
1:D:343:ASN:HB2	1:D:386:ILE:HD13	1.78	0.66
1:N:356:GLU:HG3	1:N:361:GLN:NE2	2.10	0.66
1:L:221:ALA:O	1:M:204:ASN:HB2	1.96	0.66
1:C:6:LEU:HB2	1:C:25:VAL:HG13	1.77	0.66
1:A:392:GLU:CG	1:A:393:GLY:N	2.59	0.65
1:I:151:GLU:HB3	1:I:152:PRO:CD	2.24	0.65
1:E:41:ASP:O	1:E:43:PRO:HD3	1.97	0.65
1:N:207:TYR:O	1:N:238:ARG:NH1	2.25	0.65
1:A:199:THR:HG21	1:G:181:GLN:NE2	2.11	0.65
1:L:6:LEU:HB2	1:L:25:VAL:HG13	1.78	0.65
1:J:343:ASN:HB2	1:J:386:ILE:HD13	1.79	0.65
1:M:58:GLY:HA2	1:M:376:VAL:HG23	1.79	0.65
1:L:377:VAL:HB	1:L:398:TYR:HB2	1.79	0.64
1:G:41:ASP:O	1:G:43:PRO:HD3	1.98	0.64
1:K:207:TYR:O	1:K:238:ARG:NH1	2.28	0.64
1:K:144:ARG:HH11	1:K:152:PRO:HD2	1.63	0.63
1:D:343:ASN:HD22	1:D:386:ILE:HB	1.63	0.63
1:A:150:LEU:O	1:A:151:GLU:HB2	1.98	0.63
1:H:41:ASP:O	1:H:43:PRO:HD3	1.99	0.63
1:I:176:VAL:HG11	1:I:218:GLU:CB	2.29	0.63
1:L:356:GLU:HA	1:L:361:GLN:HE21	1.63	0.63
1:A:271:THR:O	1:A:274:THR:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:VAL:HB	1:D:398:TYR:HB2	1.82	0.62
1:D:239:ALA:O	1:D:244:VAL:HG13	1.99	0.62
1:F:6:LEU:HB2	1:F:25:VAL:HG13	1.80	0.62
1:I:192:SER:HB3	1:I:230:ALA:HA	1.82	0.62
1:F:41:ASP:O	1:F:43:PRO:HD3	2.00	0.62
1:J:207:TYR:O	1:J:238:ARG:NH1	2.30	0.62
1:I:176:VAL:HG11	1:I:218:GLU:HB3	1.82	0.61
1:J:204:ASN:HB2	1:P:221:ALA:O	2.00	0.61
1:D:41:ASP:O	1:D:43:PRO:HD3	1.99	0.61
1:K:58:GLY:HA2	1:K:376:VAL:HG23	1.81	0.61
1:O:103:VAL:HG22	1:O:125:PRO:HB2	1.81	0.61
1:L:382:PRO:HA	1:L:385:ASP:O	2.00	0.61
1:A:41:ASP:O	1:A:43:PRO:HD3	2.00	0.61
1:J:10:ASN:HD22	1:J:21:GLU:HA	1.66	0.61
1:B:136:GLN:HG2	3:B:447:HOH:O	2.01	0.61
1:E:181:GLN:NE2	1:H:199:THR:HG21	2.16	0.61
1:G:56:MET:HE1	1:G:347:LEU:HD22	1.83	0.61
1:N:6:LEU:HB2	1:N:25:VAL:HG13	1.83	0.61
1:O:6:LEU:HB2	1:O:25:VAL:HG13	1.83	0.60
1:C:204:ASN:ND2	3:C:430:HOH:O	2.34	0.60
1:D:6:LEU:HB2	1:D:25:VAL:HG13	1.83	0.60
1:G:6:LEU:HB2	1:G:25:VAL:HG13	1.82	0.60
1:K:378:LEU:HD21	1:K:389:VAL:HG22	1.82	0.60
1:M:347:LEU:HD11	1:M:382:PRO:HB2	1.82	0.60
1:B:6:LEU:HB2	1:B:25:VAL:HG13	1.84	0.59
1:K:41:ASP:O	1:K:43:PRO:HD3	2.02	0.59
1:K:6:LEU:HB2	1:K:25:VAL:HG13	1.85	0.59
1:P:207:TYR:O	1:P:238:ARG:NH1	2.28	0.59
1:A:204:ASN:HB3	1:G:223:ASN:ND2	2.18	0.59
1:C:182:LYS:HD3	1:F:150:LEU:HD23	1.84	0.59
1:I:343:ASN:HB2	1:I:386:ILE:HD13	1.84	0.59
1:F:40:VAL:HG13	1:F:42:LEU:CD2	2.33	0.59
1:F:40:VAL:HG13	1:F:42:LEU:HD23	1.84	0.59
1:L:236:ILE:HG21	1:L:261:MET:HE2	1.84	0.59
1:N:347:LEU:HD11	1:N:382:PRO:HB2	1.84	0.59
1:H:31:ARG:NH2	1:H:370:GLY:O	2.36	0.58
1:H:263:GLU:HB3	1:M:39:PRO:HG3	1.85	0.58
1:J:343:ASN:HD22	1:J:386:ILE:HB	1.68	0.58
1:L:325:GLU:CD	1:L:325:GLU:H	2.11	0.58
1:J:57:PRO:HG3	1:J:367:ILE:HG13	1.86	0.58
1:K:10:ASN:HD22	1:K:21:GLU:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:41:ASP:O	1:J:43:PRO:HD3	2.04	0.58
1:K:377:VAL:HB	1:K:398:TYR:HB2	1.86	0.58
1:F:61:ASP:OD2	1:F:320[A]:SER:OG	2.21	0.58
1:A:299:GLN:HG3	1:A:300:GLN:HE21	1.67	0.57
1:F:140:HIS:CE1	1:F:194:GLY:HA3	2.39	0.57
1:J:199:THR:HG21	1:P:181:GLN:NE2	2.18	0.57
1:O:41:ASP:O	1:O:43:PRO:HD3	2.04	0.57
1:E:6:LEU:HB2	1:E:25:VAL:HG13	1.87	0.57
1:A:153:CYS:SG	1:A:154:SER:N	2.78	0.57
1:B:181:GLN:NE2	1:D:199:THR:HG21	2.19	0.57
1:N:103:VAL:HG22	1:N:125:PRO:HB2	1.86	0.57
1:P:261:MET:HG2	1:P:266:ALA:HB3	1.86	0.57
1:B:215:ILE:HG22	1:B:226:VAL:HG21	1.86	0.56
1:D:303:ARG:NH2	1:D:339:GLU:OE1	2.38	0.56
1:P:64:VAL:HG21	1:P:103:VAL:HB	1.87	0.56
1:B:154:SER:OG	1:B:155:CYS:N	2.36	0.56
1:J:379:ASP:HB3	1:J:395:ARG:HG2	1.86	0.56
1:A:58:GLY:HA2	1:A:376:VAL:HG23	1.88	0.56
1:A:392:GLU:HG2	1:A:393:GLY:H	1.70	0.56
1:G:388:VAL:HA	1:G:395:ARG:HE	1.71	0.56
1:N:58:GLY:HA2	1:N:376:VAL:HG23	1.87	0.56
1:D:10:ASN:HD22	1:D:21:GLU:HA	1.70	0.56
1:L:207:TYR:O	1:L:238:ARG:NH1	2.35	0.56
1:D:140:HIS:CE1	1:D:194:GLY:HA3	2.41	0.56
1:P:10:ASN:HD22	1:P:21:GLU:HA	1.70	0.56
1:B:16:ARG:HH12	1:B:20:LEU:HD21	1.71	0.56
1:M:41:ASP:O	1:M:43:PRO:HD3	2.05	0.56
1:L:32:ILE:HD13	1:L:367:ILE:HG23	1.88	0.56
1:I:82:ILE:CD1	1:J:112:SER:HB2	2.36	0.55
1:K:16:ARG:HH12	1:K:20:LEU:HD21	1.69	0.55
1:A:388:VAL:HA	1:A:395:ARG:HH11	1.71	0.55
1:C:58:GLY:HA2	1:C:376:VAL:HG23	1.89	0.55
1:N:10:ASN:HD22	1:N:21:GLU:HA	1.71	0.55
1:O:347:LEU:HD11	1:O:382:PRO:HB2	1.88	0.55
1:A:10:ASN:HD22	1:A:21:GLU:HA	1.72	0.55
1:F:261:MET:HG2	1:F:266:ALA:HB3	1.89	0.55
1:H:61:ASP:HB3	1:H:103:VAL:HG12	1.89	0.55
1:H:263:GLU:HB3	1:M:39:PRO:CG	2.36	0.55
1:L:154:SER:O	1:L:155:CYS:CB	2.50	0.55
1:I:65:HIS:CE1	1:I:106:ALA:HB3	2.42	0.55
1:D:223:ASN:ND2	1:E:204[A]:ASN:OD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:41:ASP:O	1:I:43:PRO:HD3	2.07	0.55
1:P:6:LEU:HB2	1:P:25:VAL:HG13	1.89	0.55
1:P:140:HIS:CE1	1:P:194:GLY:HA3	2.42	0.55
1:H:89:LEU:HB2	1:H:90:PRO:HD3	1.87	0.55
1:E:10:ASN:HD22	1:E:21:GLU:HA	1.71	0.54
1:M:16:ARG:HH12	1:M:20:LEU:HD21	1.73	0.54
1:J:378:LEU:HD21	1:J:389:VAL:HG22	1.88	0.54
1:N:140:HIS:CE1	1:N:194:GLY:HA3	2.43	0.54
1:C:206:GLN:O	1:C:207:TYR:HB2	2.07	0.54
1:H:150:LEU:HD23	1:H:152:PRO:HD2	1.90	0.54
1:N:221:ALA:O	1:O:204:ASN:HB2	2.08	0.54
1:E:144:ARG:HD2	1:E:151:GLU:HB3	1.88	0.54
1:E:234:ARG:O	1:E:238:ARG:HG2	2.08	0.54
1:I:151:GLU:OE2	1:I:151:GLU:HA	2.07	0.54
1:A:6:LEU:HB2	1:A:25:VAL:HG13	1.89	0.54
1:A:199:THR:HG21	1:G:181:GLN:HE21	1.72	0.54
1:P:82:ILE:O	1:P:86:ILE:HG12	2.07	0.54
1:G:173:ARG:NH2	3:G:434:HOH:O	2.41	0.53
1:D:287:MET:HE3	1:D:292:VAL:HG22	1.89	0.53
1:M:82:ILE:O	1:M:86:ILE:HG12	2.07	0.53
1:A:221:ALA:O	1:C:204:ASN:HB2	2.08	0.53
1:G:82:ILE:O	1:G:86:ILE:HG12	2.09	0.53
1:H:82:ILE:O	1:H:86:ILE:HG12	2.09	0.53
1:I:16:ARG:HH12	1:I:20:LEU:HD21	1.74	0.53
1:J:223:ASN:ND2	1:L:204:ASN:HB3	2.24	0.53
1:N:192:SER:CB	1:N:230:ALA:HA	2.39	0.53
1:C:37:ASP:OD1	1:C:37:ASP:N	2.41	0.53
1:M:201:PRO:O	1:M:204:ASN:ND2	2.42	0.53
1:M:249:HIS:HE1	1:M:321:ASP:OD2	1.92	0.53
1:P:299:GLN:HG3	1:P:300:GLN:HE21	1.74	0.53
1:A:61:ASP:OD2	1:A:320[A]:SER:OG	2.24	0.53
1:G:343:ASN:HB2	1:G:386:ILE:HD13	1.89	0.53
1:A:170:GLU:OE2	1:A:170:GLU:HA	2.08	0.52
1:E:201:PRO:HG2	1:E:204[A]:ASN:ND2	2.24	0.52
1:E:98:ARG:NH2	3:E:427:HOH:O	2.41	0.52
1:B:132:LYS:HE3	1:B:161:ALA:O	2.09	0.52
1:H:129:PRO:HD2	1:H:185:THR:HG23	1.90	0.52
1:O:65:HIS:CD2	1:O:321:ASP:OD1	2.62	0.52
1:L:103:VAL:HG22	1:L:125:PRO:HB2	1.91	0.52
1:B:16:ARG:HD2	1:N:51:ARG:CG	2.39	0.52
1:O:393:GLY:O	1:O:395:ARG:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HB2	1:B:189:ILE:HG22	1.92	0.52
1:C:47:ALA:C	1:C:48:ILE:HG13	2.35	0.52
1:J:58:GLY:HA2	1:J:376:VAL:HG23	1.91	0.52
1:N:378:LEU:HD21	1:N:389:VAL:HG22	1.92	0.52
1:P:72:ASN:HB3	1:P:75:VAL:HG12	1.92	0.52
1:L:378:LEU:HD21	1:L:389:VAL:HG22	1.92	0.52
1:N:261:MET:HG2	1:N:266:ALA:HB3	1.91	0.52
1:O:61:ASP:OD2	1:O:320:SER:OG	2.27	0.52
1:A:249:HIS:HE1	1:A:321:ASP:OD2	1.93	0.51
1:P:204:ASN:C	1:P:204:ASN:HD22	2.17	0.51
1:G:194:GLY:HA2	1:G:231:TYR:HE2	1.75	0.51
1:I:58:GLY:HA2	1:I:376:VAL:HG23	1.91	0.51
1:M:267:PHE:N	1:M:267:PHE:CD2	2.79	0.51
1:F:270:PRO:O	1:F:337:ARG:NH2	2.44	0.51
1:N:13:ASP:OD1	1:N:16:ARG:HD3	2.10	0.51
1:N:338:ALA:HB1	1:N:343:ASN:HB3	1.92	0.51
1:N:146:ARG:HH21	1:N:199:THR:HB	1.75	0.51
1:N:154:SER:O	1:N:155:CYS:CB	2.58	0.51
1:C:82:ILE:O	1:C:86:ILE:HG12	2.10	0.51
1:C:388:VAL:HA	1:C:395:ARG:HH11	1.76	0.51
1:K:60:ILE:HG12	1:K:102:SER:HB2	1.92	0.51
1:M:325:GLU:CD	1:M:325:GLU:H	2.18	0.51
1:P:151:GLU:CB	1:P:152:PRO:HD3	2.39	0.51
1:F:129:PRO:HD2	1:F:185:THR:HG23	1.92	0.51
1:F:223:ASN:ND2	1:G:204:ASN:HB3	2.26	0.51
1:I:379:ASP:HB3	1:I:395:ARG:HG2	1.92	0.51
1:E:88:SER:HA	1:E:91:ILE:HD12	1.92	0.51
1:H:271:THR:O	1:H:274:THR:HG22	2.11	0.51
1:L:41:ASP:O	1:L:43:PRO:HD3	2.10	0.51
1:L:347:LEU:HD11	1:L:382:PRO:HB2	1.93	0.51
1:C:31:ARG:NH2	1:C:370:GLY:O	2.43	0.51
1:K:236:ILE:O	1:K:240:VAL:HG23	2.11	0.51
1:N:393:GLY:C	1:N:395:ARG:H	2.18	0.51
1:B:181:GLN:HE21	1:D:199:THR:HG21	1.76	0.50
1:C:223:ASN:ND2	1:F:204:ASN:HB3	2.27	0.50
1:K:271:THR:O	1:K:274:THR:HG22	2.12	0.50
1:L:10:ASN:HD22	1:L:21:GLU:HA	1.75	0.50
1:L:236:ILE:O	1:L:240:VAL:HG23	2.12	0.50
1:L:356:GLU:HA	1:L:361:GLN:NE2	2.25	0.50
1:M:60:ILE:HG12	1:M:102:SER:HB2	1.92	0.50
1:N:146:ARG:HG2	1:N:147:GLY:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:181:GLN:NE2	1:P:199:THR:HG21	2.26	0.50
1:H:10:ASN:HD22	1:H:21:GLU:HA	1.76	0.50
1:L:206:GLN:O	1:L:207:TYR:HB2	2.11	0.50
1:C:61:ASP:HB3	1:C:103:VAL:HG12	1.94	0.50
1:F:49:ASP:OD1	1:F:51:ARG:NH1	2.45	0.50
1:G:249:HIS:HE1	1:G:321:ASP:OD2	1.94	0.50
1:P:41:ASP:O	1:P:43:PRO:HD3	2.12	0.50
1:E:160:GLY:N	3:E:424:HOH:O	2.44	0.49
1:H:173:ARG:HG2	1:H:218:GLU:HG3	1.93	0.49
1:C:201:PRO:HG2	1:C:204:ASN:OD1	2.13	0.49
1:J:299:GLN:HG3	1:J:300:GLN:HE21	1.76	0.49
1:M:170:GLU:OE2	1:M:170:GLU:HA	2.12	0.49
1:L:173:ARG:O	1:L:177:ARG:HG3	2.13	0.49
1:C:347:LEU:HD11	1:C:382:PRO:HB2	1.95	0.49
1:D:261:MET:HG2	1:D:266:ALA:HB3	1.93	0.49
1:G:270:PRO:O	1:G:337:ARG:NH2	2.45	0.49
1:I:361:GLN:CD	1:I:361:GLN:H	2.21	0.49
1:P:378:LEU:HD21	1:P:389:VAL:HG22	1.93	0.49
1:A:392:GLU:HG3	1:A:393:GLY:N	2.24	0.49
1:C:271:THR:O	1:C:274:THR:HG22	2.12	0.49
1:D:89:LEU:HB2	1:D:90:PRO:HD3	1.94	0.49
1:E:343:ASN:HD22	1:E:386:ILE:HB	1.78	0.49
1:H:88:SER:HA	1:H:91:ILE:HD12	1.93	0.49
1:I:201:PRO:O	1:I:204:ASN:ND2	2.46	0.49
1:M:373:ALA:HB3	1:M:403:GLY:H	1.78	0.49
1:B:240:VAL:HG21	1:B:261:MET:HG3	1.95	0.49
1:E:379:ASP:HB3	1:E:395:ARG:HG2	1.94	0.49
1:I:60:ILE:HB	1:I:354:ALA:HB1	1.95	0.49
1:I:299:GLN:HG3	1:I:300:GLN:HE21	1.78	0.49
1:A:261:MET:HG2	1:A:266:ALA:HB3	1.95	0.49
1:B:261:MET:HG2	1:B:266:ALA:HB3	1.94	0.49
1:D:344:LEU:HD13	1:D:348:ARG:NH1	2.27	0.49
1:F:82:ILE:O	1:F:86:ILE:HG12	2.13	0.49
1:J:170:GLU:OE2	1:J:170:GLU:HA	2.12	0.49
1:B:199:THR:HG21	1:H:181:GLN:NE2	2.28	0.49
1:F:49:ASP:OD1	1:F:51:ARG:HG3	2.12	0.49
1:I:176:VAL:HG11	1:I:218:GLU:HB2	1.95	0.49
1:N:168:GLY:O	1:N:172:VAL:HG22	2.13	0.49
1:D:144:ARG:HD2	1:D:151:GLU:HB3	1.94	0.48
1:D:344:LEU:HD13	1:D:348:ARG:HH12	1.78	0.48
1:F:146:ARG:HH21	1:F:199:THR:HB	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:347:LEU:HD11	1:H:382:PRO:HB2	1.95	0.48
1:J:347:LEU:HD11	1:J:382:PRO:HB2	1.95	0.48
1:E:206:GLN:O	1:E:207:TYR:HB2	2.12	0.48
1:H:92:LEU:HD22	1:H:125:PRO:HD2	1.95	0.48
1:L:188:LYS:HD3	1:L:227:MET:HE2	1.95	0.48
1:A:88:SER:HA	1:A:91:ILE:HD12	1.93	0.48
1:B:113:LEU:HA	1:B:113:LEU:HD23	1.69	0.48
1:B:173:ARG:HG2	1:B:218:GLU:HG3	1.95	0.48
1:D:76:ASN:O	1:D:79:GLN:HG2	2.13	0.48
1:O:261:MET:HG2	1:O:266:ALA:HB3	1.96	0.48
1:I:31:ARG:NH2	1:I:370:GLY:O	2.46	0.48
1:K:379:ASP:HB3	1:K:395:ARG:HG2	1.95	0.48
1:M:261:MET:HE1	1:M:309:TYR:HE1	1.79	0.48
1:P:343:ASN:HB2	1:P:386:ILE:HD13	1.96	0.48
1:E:236:ILE:HG21	1:E:261:MET:HE2	1.94	0.48
1:F:325:GLU:H	1:F:325:GLU:CD	2.20	0.48
1:M:271:THR:O	1:M:274:THR:HG22	2.13	0.48
1:I:221:ALA:O	1:K:204:ASN:CB	2.48	0.48
1:J:61:ASP:OD1	1:J:319:GLY:HA2	2.12	0.48
1:P:61:ASP:HB3	1:P:103:VAL:HG12	1.96	0.48
1:N:41:ASP:O	1:N:43:PRO:HD3	2.13	0.48
1:P:250:GLY:O	1:P:253:VAL:HG22	2.13	0.48
1:A:140:HIS:CE1	1:A:194:GLY:HA3	2.48	0.48
1:I:10:ASN:HD22	1:I:21:GLU:HA	1.78	0.48
1:O:129:PRO:HD2	1:O:185:THR:HG23	1.96	0.48
1:A:103:VAL:HG22	1:A:125:PRO:HB2	1.96	0.47
1:B:61:ASP:OD2	1:B:320[A]:SER:OG	2.27	0.47
1:F:240:VAL:HG21	1:F:261:MET:HG3	1.96	0.47
1:H:280:LYS:HB3	1:H:281:HIS:CE1	2.49	0.47
1:A:89:LEU:HB2	1:A:90:PRO:HD3	1.95	0.47
1:B:140:HIS:ND1	1:B:194:GLY:HA3	2.29	0.47
1:C:173:ARG:HG2	1:C:218:GLU:HG3	1.96	0.47
1:H:204:ASN:C	1:H:204:ASN:HD22	2.23	0.47
1:I:236:ILE:HG21	1:I:261:MET:HE2	1.94	0.47
1:O:88:SER:HA	1:O:91:ILE:HD12	1.95	0.47
1:C:177:ARG:NH2	1:F:211:GLU:OE2	2.37	0.47
1:M:153:CYS:O	1:M:154:SER:CB	2.57	0.47
1:O:236:ILE:O	1:O:240:VAL:HG23	2.14	0.47
1:O:270:PRO:O	1:O:337:ARG:NH2	2.47	0.47
1:E:271:THR:HG21	1:E:321:ASP:HB2	1.95	0.47
1:I:6:LEU:HB2	1:I:25:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:82:ILE:HD13	1:J:112:SER:HB2	1.97	0.47
1:O:31:ARG:NH2	1:O:370:GLY:O	2.45	0.47
1:G:261:MET:HG2	1:G:266:ALA:HB3	1.96	0.47
1:M:356:GLU:HG3	1:M:361:GLN:HE21	1.79	0.47
1:C:16:ARG:HH12	1:C:20:LEU:HD21	1.80	0.47
1:G:187:ILE:HB	1:G:226:VAL:HG22	1.95	0.47
1:G:239:ALA:O	1:G:244:VAL:HG13	2.15	0.47
1:C:10:ASN:HD22	1:C:21:GLU:HA	1.78	0.47
1:J:258:ALA:HA	1:J:261:MET:HE3	1.96	0.47
1:J:373:ALA:HB3	1:J:403:GLY:H	1.80	0.47
1:O:140:HIS:CE1	1:O:194:GLY:HA3	2.50	0.47
1:P:288:PRO:HA	1:P:289:PRO:HD3	1.80	0.47
1:A:270:PRO:O	1:A:337:ARG:NH2	2.47	0.47
1:I:271:THR:O	1:I:274:THR:HG22	2.14	0.47
1:L:224:THR:OG1	1:L:225:TYR:N	2.41	0.47
1:O:172:VAL:O	1:O:176:VAL:HG23	2.15	0.47
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.14	0.47
1:M:379:ASP:HB3	1:M:395:ARG:HG2	1.96	0.47
1:N:303:ARG:HG2	1:N:340:VAL:HG21	1.97	0.47
1:P:53:LYS:HG2	1:P:379:ASP:HA	1.97	0.47
1:A:152:PRO:O	1:A:153:CYS:HB3	2.14	0.47
1:C:338:ALA:O	1:C:341:LEU:O	2.32	0.47
1:E:270:PRO:HD2	1:E:337:ARG:HH22	1.80	0.47
1:L:318:PHE:CZ	1:L:333:GLU:HB3	2.50	0.46
1:C:258:ALA:HA	1:C:261:MET:HE3	1.96	0.46
1:D:51:ARG:HD2	1:D:51:ARG:O	2.15	0.46
1:G:261:MET:HE1	1:G:309:TYR:HE1	1.80	0.46
1:H:170:GLU:OE2	1:H:170:GLU:HA	2.14	0.46
1:I:325:GLU:C	1:I:327:HIS:H	2.23	0.46
1:J:103:VAL:HG22	1:J:125:PRO:HB2	1.95	0.46
1:K:388:VAL:HA	1:K:395:ARG:HH11	1.81	0.46
1:N:82:ILE:O	1:N:86:ILE:HG12	2.15	0.46
1:I:388:VAL:HA	1:I:395:ARG:HH11	1.79	0.46
1:M:236:ILE:HG21	1:M:261:MET:HE2	1.97	0.46
1:N:236:ILE:HG21	1:N:261:MET:HE2	1.97	0.46
1:A:194:GLY:HA2	1:A:231:TYR:HE2	1.80	0.46
1:B:192:SER:HB3	1:B:230:ALA:HA	1.97	0.46
1:G:347:LEU:HD11	1:G:382:PRO:HB2	1.97	0.46
1:B:140:HIS:CE1	1:B:194:GLY:HA3	2.51	0.46
1:E:61:ASP:HB3	1:E:103:VAL:HG12	1.97	0.46
1:C:44:ASN:H	1:C:44:ASN:HD22	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ARG:NH2	3:D:429:HOH:O	2.30	0.46
1:M:236:ILE:HD11	1:M:250:GLY:HA2	1.97	0.46
1:N:61:ASP:HB3	1:N:103:VAL:HG12	1.98	0.46
1:F:299:GLN:HG3	1:F:300:GLN:HE21	1.81	0.46
1:H:388:VAL:HA	1:H:395:ARG:HH11	1.80	0.46
1:K:104:ARG:HA	1:K:128:PHE:HB2	1.98	0.46
1:D:240:VAL:HG21	1:D:261:MET:HG3	1.98	0.46
1:F:170:GLU:OE2	1:F:170:GLU:HA	2.16	0.46
1:G:236:ILE:HG21	1:G:261:MET:HE2	1.98	0.46
1:K:7:GLN:NE2	1:K:47:ALA:HB1	2.31	0.46
1:K:65:HIS:CE1	1:K:106:ALA:HB3	2.51	0.46
1:L:61:ASP:HB3	1:L:103:VAL:HG12	1.98	0.46
1:M:267:PHE:HD2	1:M:267:PHE:H	1.63	0.46
1:N:236:ILE:HD13	1:N:253:VAL:HG13	1.97	0.46
1:G:153:CYS:SG	1:G:154:SER:N	2.89	0.46
1:E:56:MET:HE1	1:E:347:LEU:HD22	1.98	0.46
1:E:393:GLY:O	1:E:395:ARG:N	2.48	0.46
1:K:325:GLU:H	1:K:325:GLU:CD	2.24	0.46
1:N:31:ARG:NH2	1:N:370:GLY:O	2.48	0.46
1:O:270:PRO:HD2	1:O:337:ARG:HH22	1.81	0.46
1:C:140:HIS:CE1	1:C:194:GLY:HA3	2.51	0.45
1:G:24:HIS:N	1:G:36:THR:O	2.47	0.45
1:H:63:HIS:ND1	1:H:248:GLU:OE1	2.34	0.45
1:I:206:GLN:O	1:I:207:TYR:HB2	2.14	0.45
1:K:221:ALA:O	1:N:204:ASN:CB	2.60	0.45
1:P:388:VAL:HA	1:P:395:ARG:HE	1.81	0.45
1:C:343:ASN:HD22	1:C:386:ILE:HB	1.80	0.45
1:D:241[A]:ARG:HG3	1:D:260:LEU:HD21	1.98	0.45
1:E:388:VAL:HA	1:E:395:ARG:HE	1.82	0.45
1:K:31:ARG:NH2	1:K:370:GLY:O	2.49	0.45
1:M:72:ASN:HB3	1:M:75:VAL:HG12	1.99	0.45
1:N:135:SER:O	1:N:165:VAL:HA	2.15	0.45
1:N:373:ALA:HB3	1:N:403:GLY:H	1.80	0.45
1:O:10:ASN:HD22	1:O:21:GLU:HA	1.82	0.45
1:B:153:CYS:O	1:B:154:SER:CB	2.59	0.45
1:C:192:SER:HB3	1:C:230:ALA:HA	1.96	0.45
1:D:173:ARG:HG2	1:D:218:GLU:CG	2.47	0.45
1:B:107:GLY:O	1:B:162:ILE:HD12	2.16	0.45
1:H:6:LEU:HB2	1:H:25:VAL:HG13	1.98	0.45
1:L:270:PRO:O	1:L:337:ARG:NH2	2.49	0.45
1:L:388:VAL:HA	1:L:395:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASN:HB2	1:A:386:ILE:HD13	1.98	0.45
1:O:381:ASN:HA	1:O:382:PRO:HD2	1.85	0.45
1:P:24:HIS:N	1:P:36:THR:O	2.46	0.45
1:A:173:ARG:HG2	1:A:218:GLU:HG3	1.99	0.45
1:H:288:PRO:HA	1:H:289:PRO:HD3	1.83	0.45
1:I:338:ALA:HB1	1:I:343:ASN:HB3	1.99	0.45
1:K:382:PRO:HA	1:K:385:ASP:O	2.16	0.45
1:L:316:MET:O	1:L:353:VAL:HG11	2.16	0.45
1:N:113:LEU:HD23	1:N:113:LEU:HA	1.75	0.45
1:B:151:GLU:N	1:B:152:PRO:CD	2.80	0.45
1:B:241:ARG:HG3	1:B:260:LEU:HD21	1.97	0.45
1:I:258:ALA:HA	1:I:261:MET:HE3	1.99	0.45
1:J:65:HIS:HE1	1:J:106:ALA:O	2.00	0.45
1:E:288:PRO:HA	1:E:289:PRO:HD3	1.81	0.45
1:J:261:MET:HE1	1:J:309:TYR:HE1	1.81	0.45
1:P:338:ALA:HB1	1:P:343:ASN:HB3	1.98	0.45
1:F:215:ILE:HG22	1:F:226:VAL:HG21	1.98	0.45
1:I:288:PRO:HA	1:I:289:PRO:HD3	1.84	0.45
1:G:10:ASN:HD22	1:G:21:GLU:HA	1.81	0.45
1:G:209:GLU:HB3	1:G:213[B]:ARG:HH21	1.82	0.45
1:L:338:ALA:HB2	1:L:386:ILE:HG12	1.99	0.45
1:C:270:PRO:O	1:C:337:ARG:NH2	2.50	0.44
1:D:58:GLY:HA2	1:D:376:VAL:HG23	1.98	0.44
1:F:388:VAL:HA	1:F:395:ARG:HH11	1.82	0.44
1:G:151:GLU:OE1	1:G:151:GLU:HA	2.18	0.44
1:I:3:ILE:HG13	1:I:27:ILE:O	2.17	0.44
1:K:151:GLU:OE2	1:K:151:GLU:HA	2.17	0.44
1:M:401:GLN:HB2	1:M:406:VAL:HG21	1.99	0.44
1:D:270:PRO:O	1:D:337:ARG:NH2	2.50	0.44
1:F:270:PRO:HD2	1:F:337:ARG:HH22	1.82	0.44
1:G:16:ARG:HH12	1:G:20:LEU:HD21	1.82	0.44
1:H:335:ARG:NH1	1:H:335:ARG:HB3	2.31	0.44
1:K:299:GLN:HG3	1:K:300:GLN:HE21	1.82	0.44
1:M:258:ALA:HA	1:M:261:MET:HE3	1.99	0.44
1:O:373:ALA:HB3	1:O:403:GLY:H	1.81	0.44
1:P:31:ARG:NH2	1:P:370:GLY:O	2.51	0.44
1:B:388:VAL:HA	1:B:395:ARG:HH11	1.82	0.44
1:C:215:ILE:HG22	1:C:226:VAL:HG21	2.00	0.44
1:I:378:LEU:HD21	1:I:389:VAL:HG22	1.99	0.44
1:I:381:ASN:HA	1:I:382:PRO:HD2	1.90	0.44
1:N:56:MET:HA	1:N:367:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:135:SER:O	1:P:165:VAL:HA	2.18	0.44
1:D:258:ALA:HA	1:D:261:MET:HE3	1.99	0.44
1:H:258:ALA:HA	1:H:261:MET:HE3	1.99	0.44
1:H:383:LEU:HD12	1:H:383:LEU:HA	1.84	0.44
1:I:104:ARG:HD3	1:I:358:VAL:HG12	2.00	0.44
1:N:288:PRO:HA	1:N:289:PRO:HD3	1.82	0.44
1:B:343:ASN:OD1	1:B:343:ASN:N	2.38	0.44
1:E:181:GLN:HE21	1:H:199:THR:HG21	1.81	0.44
1:K:172:VAL:O	1:K:176:VAL:HG23	2.18	0.44
1:M:377:VAL:HG11	1:M:398:TYR:HD2	1.82	0.44
1:N:388:VAL:HA	1:N:395:ARG:HH11	1.82	0.44
1:F:268:VAL:HG23	1:F:314:VAL:HG12	1.99	0.44
1:I:270:PRO:O	1:I:337:ARG:NH2	2.50	0.44
1:I:347:LEU:HD11	1:I:382:PRO:HB2	2.00	0.44
1:L:272:LEU:HD11	1:L:306:LEU:HD13	2.00	0.44
1:B:10:ASN:HD22	1:B:21:GLU:HA	1.83	0.44
1:G:325:GLU:C	1:G:327:HIS:H	2.26	0.44
1:O:60:ILE:HG12	1:O:102:SER:HB2	2.00	0.44
1:B:236:ILE:HD11	1:B:250:GLY:HA2	2.00	0.44
1:E:229:HIS:ND1	1:E:249:HIS:CD2	2.86	0.44
1:I:199:THR:HG21	1:O:181:GLN:NE2	2.33	0.44
1:I:297:SER:O	1:I:300:GLN:HG2	2.17	0.44
1:K:335:ARG:HD2	1:K:390:ALA:HB3	1.99	0.44
1:H:173:ARG:HG2	1:H:218:GLU:CG	2.46	0.43
1:I:103:VAL:HG22	1:I:125:PRO:HB2	2.00	0.43
1:I:236:ILE:HD13	1:I:253:VAL:HG13	2.00	0.43
1:L:250:GLY:O	1:L:253:VAL:HG22	2.18	0.43
1:M:65:HIS:CD2	1:M:321:ASP:OD1	2.71	0.43
1:M:172:VAL:O	1:M:176:VAL:HG23	2.18	0.43
1:N:89:LEU:HB2	1:N:90:PRO:HD3	1.99	0.43
1:O:61:ASP:HB3	1:O:103:VAL:HG12	2.00	0.43
1:P:64:VAL:CG2	1:P:103:VAL:HB	2.48	0.43
1:B:150:LEU:O	1:B:151:GLU:HB2	2.18	0.43
1:D:292:VAL:O	1:D:295:VAL:HG12	2.18	0.43
1:E:61:ASP:OD2	1:E:320:SER:OG	2.31	0.43
1:E:361:GLN:CD	1:E:361:GLN:H	2.27	0.43
1:E:383:LEU:HD12	1:E:383:LEU:HA	1.84	0.43
1:J:7:GLN:NE2	1:J:47:ALA:HB1	2.33	0.43
1:M:88:SER:HA	1:M:91:ILE:HD12	1.99	0.43
1:A:261:MET:HE1	1:A:309:TYR:HE1	1.83	0.43
1:B:173:ARG:HG2	1:B:218:GLU:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:LEU:HD11	1:G:86:ILE:HD12	1.99	0.43
1:D:299:GLN:HG3	1:D:300:GLN:HE21	1.83	0.43
1:G:268:VAL:HG21	1:G:309:TYR:CE1	2.53	0.43
1:H:107:GLY:O	1:H:162:ILE:HD12	2.18	0.43
1:I:303:ARG:HH11	1:I:303:ARG:HB2	1.83	0.43
1:L:58:GLY:HA2	1:L:376:VAL:HG23	2.00	0.43
1:A:381:ASN:HA	1:A:382:PRO:HD2	1.87	0.43
1:B:88:SER:HA	1:B:91:ILE:HD12	2.00	0.43
1:C:38:ARG:O	1:C:39:PRO:C	2.62	0.43
1:D:288:PRO:HA	1:D:289:PRO:HD3	1.77	0.43
1:G:258:ALA:HA	1:G:261:MET:HE3	2.00	0.43
1:I:138:GLY:HA2	1:O:181:GLN:HG3	1.99	0.43
1:P:132:LYS:HE3	1:P:161:ALA:O	2.17	0.43
1:P:236:ILE:HG21	1:P:261:MET:CE	2.47	0.43
1:F:258:ALA:HA	1:F:261:MET:HE3	2.00	0.43
1:J:89:LEU:HB2	1:J:90:PRO:HD3	2.00	0.43
1:K:154:SER:O	1:K:155:CYS:CB	2.67	0.43
1:M:168:GLY:O	1:M:172:VAL:HG22	2.19	0.43
1:M:299:GLN:HG3	1:M:300:GLN:HE21	1.84	0.43
1:N:201:PRO:O	1:N:204:ASN:ND2	2.52	0.43
1:G:64:VAL:HG21	1:G:103:VAL:HB	2.01	0.43
1:G:271:THR:O	1:G:274:THR:HG22	2.19	0.43
1:I:153:CYS:HB2	1:I:154:SER:H	1.60	0.43
1:J:382:PRO:HA	1:J:385:ASP:O	2.19	0.43
1:M:10:ASN:HD22	1:M:21:GLU:HA	1.84	0.43
1:O:114:MET:HE3	1:O:127:ILE:O	2.18	0.43
1:G:58:GLY:HA2	1:G:376:VAL:HG23	2.01	0.43
1:G:378:LEU:HD12	1:G:378:LEU:HA	1.88	0.43
1:M:61:ASP:HB3	1:M:103:VAL:HG12	1.99	0.43
1:N:211:GLU:O	1:N:215:ILE:HG13	2.17	0.43
1:N:356:GLU:HG3	1:N:361:GLN:HE22	1.83	0.43
1:P:134:LEU:HB2	1:P:189:ILE:HG22	2.00	0.43
1:M:6:LEU:HB2	1:M:25:VAL:CG1	2.43	0.43
1:P:151:GLU:HB3	1:P:152:PRO:HD3	2.00	0.43
1:C:325:GLU:C	1:C:327:HIS:H	2.26	0.43
1:I:82:ILE:HD12	1:J:112:SER:HB2	1.99	0.43
1:I:158:ARG:H	1:I:158:ARG:HG2	1.62	0.43
1:I:261:MET:HE1	1:I:309:TYR:HE1	1.84	0.43
1:L:16:ARG:HH12	1:L:20:LEU:HD21	1.84	0.43
1:C:343:ASN:HB2	1:C:386:ILE:HD13	2.00	0.43
1:D:132:LYS:HE3	1:D:161:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:THR:HG23	3:E:434:HOH:O	2.17	0.43
1:H:151:GLU:HB3	1:H:152:PRO:CD	2.48	0.43
1:K:89:LEU:HB2	1:K:90:PRO:HD3	2.01	0.43
1:B:150:LEU:O	1:B:151:GLU:CB	2.67	0.42
1:E:58:GLY:HA2	1:E:376:VAL:HG23	2.01	0.42
1:F:232:THR:HA	1:F:252:LEU:HB2	2.01	0.42
1:J:388:VAL:HA	1:J:395:ARG:HH11	1.84	0.42
1:B:270:PRO:O	1:B:337:ARG:NH2	2.52	0.42
1:L:65:HIS:CD2	1:L:321:ASP:OD1	2.72	0.42
1:N:181:GLN:NE2	1:O:199:THR:HG21	2.33	0.42
1:N:223:ASN:HD22	1:O:204:ASN:HB3	1.83	0.42
1:N:303:ARG:HH11	1:N:303:ARG:HB2	1.84	0.42
1:O:318:PHE:CZ	1:O:333:GLU:HB3	2.54	0.42
1:A:117:VAL:HG12	1:A:122:VAL:HG12	1.99	0.42
1:E:343:ASN:HB2	1:E:386:ILE:HD13	2.02	0.42
1:I:57:PRO:HG3	1:I:367:ILE:HG13	2.00	0.42
1:I:154:SER:O	1:I:155:CYS:HB2	2.19	0.42
1:M:103:VAL:HG22	1:M:125:PRO:HB2	2.00	0.42
1:O:61:ASP:OD1	1:O:319:GLY:HA2	2.20	0.42
1:P:268:VAL:HG21	1:P:309:TYR:CE1	2.54	0.42
1:C:117:VAL:HG12	1:C:122:VAL:HG12	2.02	0.42
1:C:150:LEU:HB3	1:C:151:GLU:H	1.53	0.42
1:E:378:LEU:HD21	1:E:389:VAL:HG22	2.01	0.42
1:I:383:LEU:HD12	1:I:383:LEU:HA	1.80	0.42
1:J:261:MET:HG2	1:J:266:ALA:HB3	2.01	0.42
1:K:268:VAL:HG21	1:K:309:TYR:CE1	2.54	0.42
1:B:61:ASP:HB3	1:B:103:VAL:HG12	2.00	0.42
1:J:288:PRO:HA	1:J:289:PRO:HD3	1.86	0.42
1:K:270:PRO:O	1:K:337:ARG:NH2	2.53	0.42
1:B:236:ILE:HG21	1:B:261:MET:HE2	2.00	0.42
1:D:382:PRO:HA	1:D:385:ASP:O	2.20	0.42
1:K:287:MET:HA	1:K:288:PRO:HD2	1.83	0.42
1:L:343:ASN:HB2	1:L:386:ILE:HD13	2.01	0.42
1:M:381:ASN:HA	1:M:382:PRO:HD2	1.88	0.42
1:P:170:GLU:OE2	1:P:170:GLU:HA	2.19	0.42
1:B:51:ARG:HD2	1:B:51:ARG:O	2.20	0.42
1:B:170:GLU:HA	1:B:170:GLU:OE2	2.20	0.42
1:C:147:GLY:HA3	1:C:150:LEU:CB	2.44	0.42
1:C:261:MET:HG2	1:C:266:ALA:HB3	2.01	0.42
1:D:236:ILE:HG21	1:D:261:MET:HE2	2.02	0.42
1:G:145:PRO:HG2	1:G:150:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:62:CYS:HA	1:N:104:ARG:HB3	2.01	0.42
1:N:299:GLN:HG3	1:N:300:GLN:HE21	1.84	0.42
1:A:236:ILE:HD13	1:A:253:VAL:HG13	2.01	0.42
1:C:38:ARG:HA	1:C:39:PRO:HD2	1.51	0.42
1:F:108:GLY:HA3	3:F:427:HOH:O	2.19	0.42
1:F:268:VAL:HG23	1:F:314:VAL:CG1	2.50	0.42
1:J:28:ASP:HB3	1:J:33:VAL:HG21	2.02	0.42
1:L:42:LEU:HB2	1:L:45:ALA:HB3	2.02	0.42
1:P:385:ASP:O	1:P:388:VAL:HG13	2.19	0.42
1:D:170:GLU:HA	1:D:170:GLU:OE2	2.20	0.42
1:H:236:ILE:HD13	1:H:253:VAL:HG13	2.02	0.42
1:J:200:ASP:HA	1:J:201:PRO:HD2	1.90	0.42
1:J:270:PRO:O	1:J:337:ARG:NH2	2.53	0.42
1:M:378:LEU:HD21	1:M:389:VAL:HG22	2.01	0.42
1:O:335:ARG:HB3	1:O:335:ARG:NH1	2.35	0.42
1:D:229:HIS:ND1	1:D:249:HIS:CD2	2.88	0.42
1:D:232:THR:HA	1:D:252:LEU:HB2	2.02	0.42
1:E:117:VAL:HG12	1:E:122:VAL:HG12	2.00	0.42
1:F:65:HIS:CD2	1:F:321:ASP:OD1	2.73	0.42
1:L:236:ILE:CG2	1:L:261:MET:HE2	2.48	0.42
1:O:56:MET:HE1	1:O:347:LEU:HD22	2.01	0.42
1:D:338:ALA:HB1	1:D:343:ASN:HB3	2.01	0.41
1:H:49:ASP:OD1	1:H:51:ARG:NH1	2.53	0.41
1:H:132:LYS:HE3	1:H:161:ALA:O	2.20	0.41
1:I:176:VAL:CG1	1:I:218:GLU:HB3	2.47	0.41
1:J:401:GLN:HB2	1:J:406:VAL:HG21	2.02	0.41
1:O:132:LYS:HE3	1:O:161:ALA:O	2.20	0.41
1:P:236:ILE:CG2	1:P:261:MET:HE2	2.46	0.41
1:D:27:ILE:HG21	1:D:403:GLY:HA2	2.02	0.41
1:G:104:ARG:HA	1:G:128:PHE:HB2	2.01	0.41
1:H:234:ARG:O	1:H:238:ARG:HG2	2.20	0.41
1:K:250:GLY:O	1:K:253:VAL:HG22	2.20	0.41
1:M:287:MET:HA	1:M:288:PRO:HD2	1.86	0.41
1:A:268:VAL:HG21	1:A:309:TYR:CD1	2.54	0.41
1:B:206:GLN:O	1:B:207:TYR:HB2	2.19	0.41
1:F:151:GLU:OE1	1:F:151:GLU:N	2.51	0.41
1:F:158:ARG:H	1:F:158:ARG:HG2	1.67	0.41
1:L:31:ARG:NH2	1:L:370:GLY:O	2.53	0.41
1:O:299:GLN:HG3	1:O:300:GLN:HE21	1.84	0.41
1:P:16:ARG:HH12	1:P:20:LEU:HD21	1.85	0.41
1:P:379:ASP:HB3	1:P:395:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:GLU:CD	1:C:325:GLU:H	2.28	0.41
1:F:250:GLY:O	1:F:253:VAL:HG22	2.20	0.41
1:H:263:GLU:OE2	1:M:39:PRO:HD2	2.20	0.41
1:H:378:LEU:HD12	1:H:378:LEU:HA	1.79	0.41
1:I:113:LEU:HD23	1:I:113:LEU:HA	1.90	0.41
1:A:382:PRO:HA	1:A:385:ASP:O	2.21	0.41
1:F:192:SER:HB3	1:F:230:ALA:HA	2.02	0.41
1:H:201:PRO:HG2	1:H:204:ASN:OD1	2.20	0.41
1:H:343:ASN:HD22	1:H:386:ILE:HB	1.86	0.41
1:I:343:ASN:HD22	1:I:386:ILE:HB	1.85	0.41
1:M:229:HIS:ND1	1:M:249:HIS:CD2	2.88	0.41
1:B:345:GLU:OE1	1:B:348:ARG:NH1	2.52	0.41
1:C:212:ILE:HA	1:C:215:ILE:HD12	2.02	0.41
1:F:287:MET:HA	1:F:288:PRO:HD2	1.85	0.41
1:H:117:VAL:HG12	1:H:122:VAL:HG12	2.02	0.41
1:K:89:LEU:HD23	1:K:89:LEU:HA	1.83	0.41
1:K:192:SER:HB3	1:K:230:ALA:HA	2.03	0.41
1:O:200:ASP:HA	1:O:201:PRO:HD2	1.90	0.41
1:E:194:GLY:HA2	1:E:231:TYR:HE2	1.86	0.41
1:E:223:ASN:ND2	1:H:204:ASN:HB3	2.36	0.41
1:I:77:ALA:HA	1:I:160:GLY:O	2.19	0.41
1:J:65:HIS:CE1	1:J:106:ALA:O	2.74	0.41
1:P:150:LEU:O	1:P:151:GLU:HB2	2.21	0.41
1:E:113:LEU:HD23	1:E:113:LEU:HA	1.82	0.41
1:F:12:LEU:HD22	1:F:14:LEU:HG	2.02	0.41
1:J:181:GLN:NE2	1:L:199:THR:HG21	2.36	0.41
1:L:201:PRO:O	1:L:204:ASN:ND2	2.54	0.41
1:M:176:VAL:HG12	1:M:180:ILE:HD12	2.02	0.41
1:N:148:ASP:N	1:N:148:ASP:OD1	2.54	0.41
1:C:383:LEU:HD12	1:C:383:LEU:HA	1.80	0.41
1:E:82:ILE:HG13	1:E:83:LEU:N	2.35	0.41
1:G:76:ASN:O	1:G:79:GLN:HG2	2.20	0.41
1:G:132:LYS:HE3	1:G:161:ALA:HB3	2.02	0.41
1:I:51:ARG:HD2	1:I:51:ARG:O	2.21	0.41
1:I:61:ASP:OD1	1:I:319:GLY:HA2	2.21	0.41
1:M:328:ALA:C	1:M:330:GLN:H	2.29	0.41
1:N:32:ILE:HD13	1:N:367:ILE:HG23	2.03	0.41
1:A:383:LEU:HD12	1:A:383:LEU:HA	1.83	0.41
1:F:194:GLY:HA2	1:F:231:TYR:HE2	1.86	0.41
1:H:325:GLU:C	1:H:327:HIS:H	2.28	0.41
1:K:83:LEU:HD13	1:K:87:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:200:ASP:HA	1:K:201:PRO:HD2	1.85	0.41
1:M:140:HIS:HE1	1:M:196:ALA:H	1.69	0.41
1:A:20:LEU:HB3	1:A:23:HIS:CE1	2.56	0.40
1:A:192:SER:HB3	1:A:230:ALA:HA	2.03	0.40
1:A:200:ASP:HA	1:A:201:PRO:HD2	1.94	0.40
1:C:173:ARG:HG2	1:C:218:GLU:CG	2.51	0.40
1:F:151:GLU:HA	1:F:152:PRO:HD3	1.85	0.40
1:H:109:ALA:N	3:H:428:HOH:O	2.53	0.40
1:H:249:HIS:HE1	1:H:321:ASP:OD2	2.05	0.40
1:I:322:LEU:HD22	1:I:326:MET:O	2.21	0.40
1:J:129:PRO:HD2	1:J:185:THR:OG1	2.21	0.40
1:K:302:GLY:O	1:K:305:SER:OG	2.38	0.40
1:M:107:GLY:O	1:M:162:ILE:HD12	2.21	0.40
1:M:113:LEU:HD23	1:M:113:LEU:HA	1.75	0.40
1:D:383:LEU:HA	1:D:383:LEU:HD12	1.76	0.40
1:E:200:ASP:HA	1:E:201:PRO:HD2	1.95	0.40
1:F:176:VAL:HG11	1:F:218:GLU:CB	2.51	0.40
1:H:113:LEU:HA	1:H:113:LEU:HD23	1.80	0.40
1:H:236:ILE:CD1	1:H:253:VAL:HG13	2.52	0.40
1:L:53:LYS:HG2	1:L:379:ASP:HA	2.03	0.40
1:M:56:MET:HE3	1:M:56:MET:HB2	1.88	0.40
1:M:268:VAL:HG21	1:M:309:TYR:CE1	2.57	0.40
1:N:343:ASN:HB2	1:N:386:ILE:HD13	2.02	0.40
1:F:61:ASP:HB3	1:F:103:VAL:HG12	2.02	0.40
1:H:140:HIS:CE1	1:H:194:GLY:HA3	2.56	0.40
1:K:38:ARG:HD3	1:K:38:ARG:HA	1.88	0.40
1:N:224:THR:OG1	1:N:225:TYR:N	2.53	0.40
1:A:135:SER:O	1:A:165:VAL:HA	2.21	0.40
1:B:271:THR:O	1:B:274:THR:HG22	2.21	0.40
1:H:381:ASN:HA	1:H:382:PRO:HD2	1.97	0.40
1:K:103:VAL:HG22	1:K:125:PRO:HB2	2.03	0.40
1:P:381:ASN:HA	1:P:382:PRO:HD2	1.90	0.40
1:B:89:LEU:HB2	1:B:90:PRO:HD3	2.03	0.40
1:B:200:ASP:HA	1:B:201:PRO:HD2	1.94	0.40
1:D:173:ARG:HG2	1:D:218:GLU:HG3	2.03	0.40
1:F:383:LEU:HD12	1:F:383:LEU:HA	1.84	0.40
1:I:325:GLU:CD	1:I:325:GLU:H	2.29	0.40
1:K:288:PRO:HA	1:K:289:PRO:HD3	1.86	0.40
1:L:170:GLU:OE2	1:M:168:GLY:HA2	2.21	0.40
1:N:42:LEU:HA	1:N:43:PRO:HD3	1.98	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ALA:O	1:I:301:LYS:NZ[1_546]	1.98	0.22

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	405/423 (96%)	385 (95%)	13 (3%)	7 (2%)	7	9
1	B	407/423 (96%)	384 (94%)	16 (4%)	7 (2%)	7	9
1	C	404/423 (96%)	380 (94%)	18 (4%)	6 (2%)	8	11
1	D	405/423 (96%)	383 (95%)	17 (4%)	5 (1%)	10	15
1	E	405/423 (96%)	378 (93%)	23 (6%)	4 (1%)	12	18
1	F	403/423 (95%)	379 (94%)	19 (5%)	5 (1%)	10	15
1	G	403/423 (95%)	380 (94%)	18 (4%)	5 (1%)	10	15
1	H	403/423 (95%)	374 (93%)	21 (5%)	8 (2%)	6	8
1	I	402/423 (95%)	374 (93%)	20 (5%)	8 (2%)	6	8
1	J	395/423 (93%)	368 (93%)	22 (6%)	5 (1%)	9	14
1	K	398/423 (94%)	369 (93%)	22 (6%)	7 (2%)	6	9
1	L	401/423 (95%)	371 (92%)	21 (5%)	9 (2%)	5	7
1	M	403/423 (95%)	378 (94%)	17 (4%)	8 (2%)	6	8
1	N	401/423 (95%)	367 (92%)	28 (7%)	6 (2%)	8	11
1	O	398/423 (94%)	373 (94%)	18 (4%)	7 (2%)	6	9
1	P	403/423 (95%)	380 (94%)	17 (4%)	6 (2%)	8	11
All	All	6436/6768 (95%)	6023 (94%)	310 (5%)	103 (2%)	7	10

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	GLU
1	A	152	PRO
1	A	153	CYS
1	B	151	GLU
1	B	152	PRO
1	B	154	SER
1	G	151	GLU
1	H	151	GLU
1	H	155	CYS
1	I	151	GLU
1	J	151	GLU
1	J	152	PRO
1	K	152	PRO
1	K	154	SER
1	L	152	PRO
1	M	154	SER
1	N	155	CYS
1	O	394	ALA
1	P	151	GLU
1	P	153	CYS
1	A	43	PRO
1	B	153	CYS
1	B	155	CYS
1	C	153	CYS
1	D	152	PRO
1	D	154	SER
1	E	43	PRO
1	E	394	ALA
1	F	43	PRO
1	G	43	PRO
1	I	43	PRO
1	I	153	CYS
1	J	153	CYS
1	L	154	SER
1	L	155	CYS
1	M	342	GLY
1	N	43	PRO
1	P	43	PRO
1	B	43	PRO
1	D	43	PRO
1	D	207	TYR
1	D	249	HIS
1	E	207	TYR

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Mol	Chain	Res	Type
1	G	152	PRO
1	H	43	PRO
1	H	153	CYS
1	I	154	SER
1	I	326	MET
1	J	43	PRO
1	K	43	PRO
1	L	43	PRO
1	M	43	PRO
1	O	43	PRO
1	O	392	GLU
1	P	207	TYR
1	A	207	TYR
1	A	249	HIS
1	A	300	GLN
1	B	249	HIS
1	C	146	ARG
1	C	249	HIS
1	E	249	HIS
1	F	249	HIS
1	G	249	HIS
1	H	249	HIS
1	I	155	CYS
1	I	249	HIS
1	I	300	GLN
1	J	300	GLN
1	K	155	CYS
1	K	342	GLY
1	L	373	ALA
1	M	146	ARG
1	M	249	HIS
1	M	300	GLN
1	N	249	HIS
1	N	300	GLN
1	O	249	HIS
1	P	249	HIS
1	C	154	SER
1	F	207	TYR
1	G	207	TYR
1	H	152	PRO
1	H	207	TYR
1	K	207	TYR

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Mol	Chain	Res	Type
1	L	207	TYR
1	L	394	ALA
1	M	207	TYR
1	M	329	PHE
1	N	148	ASP
1	P	300	GLN
1	C	39	PRO
1	F	300	GLN
1	H	300	GLN
1	K	153	CYS
1	L	300	GLN
1	N	207	TYR
1	O	207	TYR
1	O	300	GLN
1	O	393	GLY
1	C	152	PRO
1	L	342	GLY
1	F	152	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/326 (97%)	263 (83%)	54 (17%)	2	2
1	B	319/326 (98%)	263 (82%)	56 (18%)	2	2
1	C	315/326 (97%)	262 (83%)	53 (17%)	2	2
1	D	317/326 (97%)	264 (83%)	53 (17%)	2	2
1	E	316/326 (97%)	267 (84%)	49 (16%)	2	2
1	F	315/326 (97%)	261 (83%)	54 (17%)	2	2
1	G	315/326 (97%)	262 (83%)	53 (17%)	2	2
1	H	315/326 (97%)	262 (83%)	53 (17%)	2	2
1	I	314/326 (96%)	262 (83%)	52 (17%)	2	2
1	J	312/326 (96%)	262 (84%)	50 (16%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	313/326 (96%)	261 (83%)	52 (17%)	2	2
1	L	313/326 (96%)	265 (85%)	48 (15%)	3	3
1	M	314/326 (96%)	261 (83%)	53 (17%)	2	2
1	N	312/326 (96%)	256 (82%)	56 (18%)	2	1
1	O	310/326 (95%)	257 (83%)	53 (17%)	2	2
1	P	315/326 (97%)	265 (84%)	50 (16%)	2	2
All	All	5032/5216 (96%)	4193 (83%)	839 (17%)	2	2

All (839) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	12	LEU
1	A	18	VAL
1	A	21	GLU
1	A	25	VAL
1	A	38	ARG
1	A	40	VAL
1	A	42	LEU
1	A	46	GLN
1	A	51	ARG
1	A	55	VAL
1	A	67	LEU
1	A	75	VAL
1	A	82	ILE
1	A	112	SER
1	A	113	LEU
1	A	122	VAL
1	A	132	LYS
1	A	151	GLU
1	A	154	SER
1	A	156	CYS
1	A	180	ILE
1	A	202	ILE
1	A	204	ASN
1	A	244	VAL
1	A	253	VAL
1	A	263	GLU
1	A	268	VAL
1	A	280	LYS

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Mol	Chain	Res	Type
1	A	292	VAL
1	A	298	VAL
1	A	306	LEU
1	A	315	LYS
1	A	320[A]	SER
1	A	320[B]	SER
1	A	325	GLU
1	A	341	LEU
1	A	344	LEU
1	A	345[A]	GLU
1	A	345[B]	GLU
1	A	361[A]	GLN
1	A	361[B]	GLN
1	A	363	GLN
1	A	375	LEU
1	A	378	LEU
1	A	383	LEU
1	A	384	GLU
1	A	388	VAL
1	A	395	ARG
1	A	396	VAL
1	A	397	GLU
1	A	404	THR
1	A	406	VAL
1	A	409	GLN
1	B	6	LEU
1	B	12	LEU
1	B	18	VAL
1	B	21	GLU
1	B	25	VAL
1	B	33	VAL
1	B	40	VAL
1	B	42	LEU
1	B	46	GLN
1	B	51	ARG
1	B	55	VAL
1	B	75	VAL
1	B	82	ILE
1	B	86	ILE
1	B	112	SER
1	B	113	LEU
1	B	122	VAL

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Mol	Chain	Res	Type
1	B	132	LYS
1	B	153	CYS
1	B	155	CYS
1	B	156	CYS
1	B	166	VAL
1	B	180	ILE
1	B	202	ILE
1	B	204	ASN
1	B	244	VAL
1	B	253	VAL
1	B	263	GLU
1	B	268	VAL
1	B	280	LYS
1	B	292	VAL
1	B	298	VAL
1	B	299	GLN
1	B	306	LEU
1	B	315	LYS
1	B	325	GLU
1	B	327[A]	HIS
1	B	327[B]	HIS
1	B	343	ASN
1	B	344	LEU
1	B	361[A]	GLN
1	B	361[B]	GLN
1	B	363	GLN
1	B	375	LEU
1	B	378	LEU
1	B	383	LEU
1	B	384	GLU
1	B	388	VAL
1	B	389	VAL
1	B	392	GLU
1	B	395	ARG
1	B	396	VAL
1	B	397	GLU
1	B	404	THR
1	B	406	VAL
1	B	409	GLN
1	C	6	LEU
1	C	12	LEU
1	C	18	VAL

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Mol	Chain	Res	Type
1	C	21	GLU
1	C	25	VAL
1	C	33	VAL
1	C	38	ARG
1	C	40	VAL
1	C	42	LEU
1	C	51	ARG
1	C	55	VAL
1	C	75	VAL
1	C	82	ILE
1	C	112	SER
1	C	113	LEU
1	C	122	VAL
1	C	150	LEU
1	C	151	GLU
1	C	155	CYS
1	C	166	VAL
1	C	180	ILE
1	C	188	LYS
1	C	202	ILE
1	C	238	ARG
1	C	246	THR
1	C	253	VAL
1	C	259	LYS
1	C	261	MET
1	C	280	LYS
1	C	292	VAL
1	C	298	VAL
1	C	299	GLN
1	C	306	LEU
1	C	315	LYS
1	C	320	SER
1	C	325	GLU
1	C	327	HIS
1	C	335	ARG
1	C	341	LEU
1	C	344	LEU
1	C	361	GLN
1	C	363	GLN
1	C	375	LEU
1	C	378	LEU
1	C	383	LEU

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Mol	Chain	Res	Type
1	C	384	GLU
1	C	388	VAL
1	C	395	ARG
1	C	396	VAL
1	C	397	GLU
1	C	404	THR
1	C	406	VAL
1	C	409	GLN
1	D	6	LEU
1	D	12	LEU
1	D	18	VAL
1	D	21	GLU
1	D	25	VAL
1	D	40	VAL
1	D	42	LEU
1	D	46	GLN
1	D	51	ARG
1	D	55	VAL
1	D	75	VAL
1	D	82	ILE
1	D	112	SER
1	D	113	LEU
1	D	121	LEU
1	D	122	VAL
1	D	123	SER
1	D	132	LYS
1	D	151	GLU
1	D	156	CYS
1	D	159	THR
1	D	166	VAL
1	D	180	ILE
1	D	188	LYS
1	D	202	ILE
1	D	238	ARG
1	D	244	VAL
1	D	253	VAL
1	D	263	GLU
1	D	268	VAL
1	D	280	LYS
1	D	292	VAL
1	D	298	VAL
1	D	299	GLN

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Mol	Chain	Res	Type
1	D	306	LEU
1	D	315	LYS
1	D	325	GLU
1	D	327	HIS
1	D	341	LEU
1	D	344	LEU
1	D	361[A]	GLN
1	D	361[B]	GLN
1	D	363	GLN
1	D	375	LEU
1	D	378	LEU
1	D	383	LEU
1	D	384	GLU
1	D	395	ARG
1	D	396	VAL
1	D	397	GLU
1	D	404	THR
1	D	406	VAL
1	D	409	GLN
1	E	6	LEU
1	E	12	LEU
1	E	18	VAL
1	E	21	GLU
1	E	25	VAL
1	E	40	VAL
1	E	46	GLN
1	E	51	ARG
1	E	55	VAL
1	E	75	VAL
1	E	82	ILE
1	E	112	SER
1	E	113	LEU
1	E	117	VAL
1	E	122	VAL
1	E	151	GLU
1	E	155	CYS
1	E	156	CYS
1	E	158	ARG
1	E	159	THR
1	E	166	VAL
1	E	202	ILE
1	E	238	ARG

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Mol	Chain	Res	Type
1	E	253	VAL
1	E	263	GLU
1	E	268	VAL
1	E	280	LYS
1	E	292	VAL
1	E	298	VAL
1	E	299	GLN
1	E	315	LYS
1	E	320	SER
1	E	325	GLU
1	E	327	HIS
1	E	341	LEU
1	E	344	LEU
1	E	361	GLN
1	E	363	GLN
1	E	375	LEU
1	E	378	LEU
1	E	383	LEU
1	E	384	GLU
1	E	388	VAL
1	E	395	ARG
1	E	396	VAL
1	E	397	GLU
1	E	404	THR
1	E	406	VAL
1	E	409	GLN
1	F	6	LEU
1	F	12	LEU
1	F	18	VAL
1	F	21	GLU
1	F	25	VAL
1	F	33	VAL
1	F	38	ARG
1	F	40	VAL
1	F	42	LEU
1	F	46	GLN
1	F	51	ARG
1	F	55	VAL
1	F	67	LEU
1	F	75	VAL
1	F	82	ILE
1	F	112	SER

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Mol	Chain	Res	Type
1	F	113	LEU
1	F	122	VAL
1	F	150	LEU
1	F	151	GLU
1	F	156	CYS
1	F	173	ARG
1	F	192	SER
1	F	202	ILE
1	F	204	ASN
1	F	238	ARG
1	F	253	VAL
1	F	261	MET
1	F	263	GLU
1	F	268	VAL
1	F	280	LYS
1	F	292	VAL
1	F	298	VAL
1	F	299	GLN
1	F	303	ARG
1	F	315	LYS
1	F	320[A]	SER
1	F	320[B]	SER
1	F	325	GLU
1	F	327	HIS
1	F	341	LEU
1	F	343	ASN
1	F	344	LEU
1	F	363	GLN
1	F	375	LEU
1	F	378	LEU
1	F	383	LEU
1	F	384	GLU
1	F	395	ARG
1	F	396	VAL
1	F	397	GLU
1	F	404	THR
1	F	406	VAL
1	F	409	GLN
1	G	3	ILE
1	G	6	LEU
1	G	12	LEU
1	G	18	VAL

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Mol	Chain	Res	Type
1	G	21	GLU
1	G	25	VAL
1	G	33	VAL
1	G	40	VAL
1	G	42	LEU
1	G	46	GLN
1	G	51	ARG
1	G	55	VAL
1	G	75	VAL
1	G	82	ILE
1	G	112	SER
1	G	113	LEU
1	G	122	VAL
1	G	150	LEU
1	G	154	SER
1	G	155	CYS
1	G	156	CYS
1	G	166	VAL
1	G	173	ARG
1	G	180	ILE
1	G	202	ILE
1	G	204	ASN
1	G	238	ARG
1	G	244	VAL
1	G	253	VAL
1	G	263	GLU
1	G	280	LYS
1	G	292	VAL
1	G	298	VAL
1	G	299	GLN
1	G	315	LYS
1	G	325	GLU
1	G	327	HIS
1	G	341	LEU
1	G	344	LEU
1	G	361	GLN
1	G	363	GLN
1	G	375	LEU
1	G	378	LEU
1	G	383	LEU
1	G	384	GLU
1	G	388	VAL

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Mol	Chain	Res	Type
1	G	392	GLU
1	G	395	ARG
1	G	396	VAL
1	G	397	GLU
1	G	404	THR
1	G	406	VAL
1	G	409	GLN
1	H	3	ILE
1	H	6	LEU
1	H	12	LEU
1	H	18	VAL
1	H	21	GLU
1	H	25	VAL
1	H	40	VAL
1	H	42	LEU
1	H	46	GLN
1	H	51	ARG
1	H	55	VAL
1	H	75	VAL
1	H	82	ILE
1	H	112	SER
1	H	113	LEU
1	H	121	LEU
1	H	122	VAL
1	H	132	LYS
1	H	136	GLN
1	H	151	GLU
1	H	166	VAL
1	H	180	ILE
1	H	190	MET
1	H	202	ILE
1	H	204	ASN
1	H	238	ARG
1	H	244	VAL
1	H	246	THR
1	H	253	VAL
1	H	261	MET
1	H	280	LYS
1	H	292	VAL
1	H	298	VAL
1	H	299	GLN
1	H	306	LEU

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Mol	Chain	Res	Type
1	H	315	LYS
1	H	325	GLU
1	H	327	HIS
1	H	341	LEU
1	H	344	LEU
1	H	361	GLN
1	H	363	GLN
1	H	375	LEU
1	H	378	LEU
1	H	383	LEU
1	H	384	GLU
1	H	388	VAL
1	H	395	ARG
1	H	396	VAL
1	H	397	GLU
1	H	404	THR
1	H	406	VAL
1	H	409	GLN
1	I	12	LEU
1	I	18	VAL
1	I	21	GLU
1	I	25	VAL
1	I	33	VAL
1	I	40	VAL
1	I	42	LEU
1	I	46	GLN
1	I	51	ARG
1	I	55	VAL
1	I	75	VAL
1	I	82	ILE
1	I	112	SER
1	I	113	LEU
1	I	121	LEU
1	I	122	VAL
1	I	132	LYS
1	I	151	GLU
1	I	153	CYS
1	I	156	CYS
1	I	173	ARG
1	I	180	ILE
1	I	192	SER
1	I	202	ILE

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Mol	Chain	Res	Type
1	I	204	ASN
1	I	238	ARG
1	I	246	THR
1	I	253	VAL
1	I	263	GLU
1	I	280	LYS
1	I	292	VAL
1	I	298	VAL
1	I	299	GLN
1	I	303	ARG
1	I	315	LYS
1	I	325	GLU
1	I	327	HIS
1	I	341	LEU
1	I	344	LEU
1	I	361	GLN
1	I	363	GLN
1	I	375	LEU
1	I	378	LEU
1	I	383	LEU
1	I	384	GLU
1	I	388	VAL
1	I	395	ARG
1	I	396	VAL
1	I	397	GLU
1	I	404	THR
1	I	406	VAL
1	I	409	GLN
1	J	3	ILE
1	J	16	ARG
1	J	18	VAL
1	J	21	GLU
1	J	25	VAL
1	J	33	VAL
1	J	40	VAL
1	J	42	LEU
1	J	46	GLN
1	J	51	ARG
1	J	55	VAL
1	J	75	VAL
1	J	82	ILE
1	J	112	SER

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Mol	Chain	Res	Type
1	J	113	LEU
1	J	122	VAL
1	J	151	GLU
1	J	156	CYS
1	J	166	VAL
1	J	173	ARG
1	J	180	ILE
1	J	192	SER
1	J	202	ILE
1	J	204	ASN
1	J	238	ARG
1	J	241	ARG
1	J	244	VAL
1	J	253	VAL
1	J	261	MET
1	J	263	GLU
1	J	280	LYS
1	J	292	VAL
1	J	298	VAL
1	J	299	GLN
1	J	315	LYS
1	J	320	SER
1	J	325	GLU
1	J	327	HIS
1	J	341	LEU
1	J	344	LEU
1	J	361	GLN
1	J	363	GLN
1	J	375	LEU
1	J	383	LEU
1	J	384	GLU
1	J	395	ARG
1	J	397	GLU
1	J	404	THR
1	J	406	VAL
1	J	409	GLN
1	K	3	ILE
1	K	6	LEU
1	K	12	LEU
1	K	14	LEU
1	K	18	VAL
1	K	21	GLU

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Mol	Chain	Res	Type
1	K	25	VAL
1	K	40	VAL
1	K	46	GLN
1	K	51	ARG
1	K	55	VAL
1	K	75	VAL
1	K	82	ILE
1	K	112	SER
1	K	113	LEU
1	K	122	VAL
1	K	132	LYS
1	K	150	LEU
1	K	156	CYS
1	K	166	VAL
1	K	180	ILE
1	K	202	ILE
1	K	204	ASN
1	K	238	ARG
1	K	253	VAL
1	K	261	MET
1	K	263	GLU
1	K	268	VAL
1	K	280	LYS
1	K	292	VAL
1	K	298	VAL
1	K	299	GLN
1	K	306	LEU
1	K	315	LYS
1	K	325	GLU
1	K	327	HIS
1	K	335	ARG
1	K	341	LEU
1	K	344	LEU
1	K	361	GLN
1	K	363	GLN
1	K	375	LEU
1	K	378	LEU
1	K	383	LEU
1	K	384	GLU
1	K	388	VAL
1	K	395	ARG
1	K	396	VAL

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Mol	Chain	Res	Type
1	K	397	GLU
1	K	404	THR
1	K	406	VAL
1	K	409	GLN
1	L	3	ILE
1	L	12	LEU
1	L	18	VAL
1	L	21	GLU
1	L	25	VAL
1	L	40	VAL
1	L	46	GLN
1	L	51	ARG
1	L	55	VAL
1	L	75	VAL
1	L	82	ILE
1	L	112	SER
1	L	113	LEU
1	L	122	VAL
1	L	126	ARG
1	L	154	SER
1	L	155	CYS
1	L	166	VAL
1	L	180	ILE
1	L	202	ILE
1	L	204	ASN
1	L	238	ARG
1	L	253	VAL
1	L	263	GLU
1	L	280	LYS
1	L	291	SER
1	L	292	VAL
1	L	298	VAL
1	L	308	ILE
1	L	315	LYS
1	L	325	GLU
1	L	327	HIS
1	L	341	LEU
1	L	344	LEU
1	L	345	GLU
1	L	361	GLN
1	L	363	GLN
1	L	375	LEU

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Mol	Chain	Res	Type
1	L	378	LEU
1	L	383	LEU
1	L	384	GLU
1	L	392	GLU
1	L	395	ARG
1	L	396	VAL
1	L	397	GLU
1	L	404	THR
1	L	406	VAL
1	L	409	GLN
1	M	6	LEU
1	M	18	VAL
1	M	21	GLU
1	M	25	VAL
1	M	33	VAL
1	M	35	VAL
1	M	40	VAL
1	M	42	LEU
1	M	46	GLN
1	M	51	ARG
1	M	55	VAL
1	M	67	LEU
1	M	75	VAL
1	M	82	ILE
1	M	112	SER
1	M	113	LEU
1	M	122	VAL
1	M	132	LYS
1	M	153	CYS
1	M	155	CYS
1	M	162	ILE
1	M	166	VAL
1	M	173	ARG
1	M	180	ILE
1	M	202	ILE
1	M	204	ASN
1	M	244	VAL
1	M	253	VAL
1	M	263	GLU
1	M	267	PHE
1	M	280	LYS
1	M	292	VAL

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Mol	Chain	Res	Type
1	M	295	VAL
1	M	298	VAL
1	M	303	ARG
1	M	306	LEU
1	M	315	LYS
1	M	325	GLU
1	M	327	HIS
1	M	335	ARG
1	M	341	LEU
1	M	344	LEU
1	M	361	GLN
1	M	363	GLN
1	M	375	LEU
1	M	383	LEU
1	M	384	GLU
1	M	395	ARG
1	M	396	VAL
1	M	397	GLU
1	M	404	THR
1	M	406	VAL
1	M	409	GLN
1	N	6	LEU
1	N	12	LEU
1	N	14	LEU
1	N	16	ARG
1	N	18	VAL
1	N	21	GLU
1	N	25	VAL
1	N	33	VAL
1	N	40	VAL
1	N	46	GLN
1	N	51	ARG
1	N	55	VAL
1	N	62	CYS
1	N	75	VAL
1	N	82	ILE
1	N	112	SER
1	N	122	VAL
1	N	132	LYS
1	N	135	SER
1	N	149	LEU
1	N	156	CYS

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Mol	Chain	Res	Type
1	N	166	VAL
1	N	180	ILE
1	N	202	ILE
1	N	204	ASN
1	N	238	ARG
1	N	253	VAL
1	N	261	MET
1	N	263	GLU
1	N	268	VAL
1	N	280	LYS
1	N	292	VAL
1	N	295	VAL
1	N	298	VAL
1	N	299	GLN
1	N	303	ARG
1	N	306	LEU
1	N	315	LYS
1	N	325	GLU
1	N	335	ARG
1	N	341	LEU
1	N	344	LEU
1	N	361	GLN
1	N	363	GLN
1	N	375	LEU
1	N	383	LEU
1	N	384	GLU
1	N	388	VAL
1	N	389	VAL
1	N	392	GLU
1	N	395	ARG
1	N	396	VAL
1	N	397	GLU
1	N	404	THR
1	N	406	VAL
1	N	409	GLN
1	O	3	ILE
1	O	12	LEU
1	O	18	VAL
1	O	21	GLU
1	O	25	VAL
1	O	33	VAL
1	O	40	VAL

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Mol	Chain	Res	Type
1	O	42	LEU
1	O	46	GLN
1	O	51	ARG
1	O	55	VAL
1	O	67	LEU
1	O	75	VAL
1	O	82	ILE
1	O	86	ILE
1	O	112	SER
1	O	113	LEU
1	O	117	VAL
1	O	122	VAL
1	O	155	CYS
1	O	156	CYS
1	O	166	VAL
1	O	173	ARG
1	O	180	ILE
1	O	202	ILE
1	O	204	ASN
1	O	238	ARG
1	O	244	VAL
1	O	253	VAL
1	O	263	GLU
1	O	280	LYS
1	O	292	VAL
1	O	298	VAL
1	O	299	GLN
1	O	303	ARG
1	O	315	LYS
1	O	325	GLU
1	O	327	HIS
1	O	341	LEU
1	O	344	LEU
1	O	361	GLN
1	O	363	GLN
1	O	375	LEU
1	O	378	LEU
1	O	383	LEU
1	O	384	GLU
1	O	388	VAL
1	O	395	ARG
1	O	396	VAL

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Mol	Chain	Res	Type
1	O	397	GLU
1	O	404	THR
1	O	406	VAL
1	O	409	GLN
1	P	3	ILE
1	P	6	LEU
1	P	12	LEU
1	P	18	VAL
1	P	21	GLU
1	P	25	VAL
1	P	40	VAL
1	P	42	LEU
1	P	46	GLN
1	P	51	ARG
1	P	55	VAL
1	P	75	VAL
1	P	82	ILE
1	P	112	SER
1	P	113	LEU
1	P	121	LEU
1	P	122	VAL
1	P	136	GLN
1	P	155	CYS
1	P	166	VAL
1	P	173	ARG
1	P	180	ILE
1	P	202	ILE
1	P	204	ASN
1	P	244	VAL
1	P	253	VAL
1	P	263	GLU
1	P	268	VAL
1	P	280	LYS
1	P	292	VAL
1	P	295	VAL
1	P	298	VAL
1	P	306	LEU
1	P	315	LYS
1	P	325	GLU
1	P	327	HIS
1	P	341	LEU
1	P	344	LEU

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Mol	Chain	Res	Type
1	P	361	GLN
1	P	363	GLN
1	P	375	LEU
1	P	383	LEU
1	P	384	GLU
1	P	388	VAL
1	P	395	ARG
1	P	396	VAL
1	P	397	GLU
1	P	404	THR
1	P	406	VAL
1	P	409	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	23	HIS
1	A	299	GLN
1	A	300	GLN
1	A	401	GLN
1	B	10	ASN
1	B	24	HIS
1	B	46	GLN
1	B	299	GLN
1	B	401	GLN
1	C	10	ASN
1	C	44	ASN
1	C	281	HIS
1	C	299	GLN
1	C	300	GLN
1	C	327	HIS
1	D	10	ASN
1	D	46	GLN
1	D	264	HIS
1	D	299	GLN
1	D	300	GLN
1	D	327	HIS
1	D	381	ASN
1	D	401	GLN
1	E	10	ASN
1	E	24	HIS

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Mol	Chain	Res	Type
1	E	46	GLN
1	E	299	GLN
1	E	300	GLN
1	E	327	HIS
1	E	401	GLN
1	F	10	ASN
1	F	24	HIS
1	F	46	GLN
1	F	204	ASN
1	F	264	HIS
1	F	281	HIS
1	F	299	GLN
1	F	300	GLN
1	F	401	GLN
1	G	10	ASN
1	G	24	HIS
1	G	46	GLN
1	G	204	ASN
1	G	299	GLN
1	G	300	GLN
1	H	10	ASN
1	H	204	ASN
1	H	299	GLN
1	H	300	GLN
1	H	361	GLN
1	H	401	GLN
1	I	10	ASN
1	I	24	HIS
1	I	46	GLN
1	I	65	HIS
1	I	204	ASN
1	I	299	GLN
1	I	300	GLN
1	I	359	ASN
1	J	10	ASN
1	J	24	HIS
1	J	65	HIS
1	J	299	GLN
1	J	300	GLN
1	J	359	ASN
1	J	363	GLN
1	J	401	GLN

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Mol	Chain	Res	Type
1	K	10	ASN
1	K	24	HIS
1	K	46	GLN
1	K	223	ASN
1	K	281	HIS
1	K	299	GLN
1	K	300	GLN
1	K	361	GLN
1	K	401	GLN
1	L	10	ASN
1	L	24	HIS
1	L	46	GLN
1	L	204	ASN
1	L	262	HIS
1	L	299	GLN
1	L	300	GLN
1	L	327	HIS
1	L	361	GLN
1	L	401	GLN
1	M	10	ASN
1	M	23	HIS
1	M	46	GLN
1	M	204	ASN
1	M	281	HIS
1	M	299	GLN
1	M	300	GLN
1	M	361	GLN
1	N	10	ASN
1	N	24	HIS
1	N	299	GLN
1	N	300	GLN
1	N	361	GLN
1	N	401	GLN
1	O	10	ASN
1	O	23	HIS
1	O	204	ASN
1	O	299	GLN
1	O	300	GLN
1	O	401	GLN
1	P	10	ASN
1	P	24	HIS
1	P	281	HIS

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Mol	Chain	Res	Type
1	P	299	GLN
1	P	300	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	405/423 (95%)	-0.07	13 (3%)	50	44	16, 50, 100, 117	4 (0%)
1	B	405/423 (95%)	-0.07	13 (3%)	50	44	11, 48, 102, 119	6 (1%)
1	C	406/423 (95%)	0.01	18 (4%)	39	32	14, 49, 104, 118	2 (0%)
1	D	405/423 (95%)	0.07	26 (6%)	25	21	14, 44, 98, 116	4 (0%)
1	E	405/423 (95%)	-0.02	11 (2%)	56	51	14, 47, 102, 119	4 (0%)
1	F	405/423 (95%)	0.00	21 (5%)	33	27	15, 49, 99, 119	2 (0%)
1	G	405/423 (95%)	-0.09	9 (2%)	62	58	13, 50, 103, 136	2 (0%)
1	H	405/423 (95%)	0.02	25 (6%)	26	22	12, 46, 100, 119	2 (0%)
1	I	405/423 (95%)	0.55	27 (6%)	24	19	28, 58, 106, 123	1 (0%)
1	J	402/423 (95%)	0.57	36 (8%)	15	12	27, 60, 103, 121	1 (0%)
1	K	403/423 (95%)	0.53	21 (5%)	33	27	25, 59, 103, 119	1 (0%)
1	L	404/423 (95%)	0.65	28 (6%)	23	19	22, 61, 106, 133	1 (0%)
1	M	406/423 (95%)	0.53	45 (11%)	10	8	23, 60, 107, 130	1 (0%)
1	N	404/423 (95%)	0.40	25 (6%)	26	22	21, 58, 106, 121	1 (0%)
1	O	401/423 (94%)	-0.02	10 (2%)	58	54	22, 53, 103, 121	1 (0%)
1	P	405/423 (95%)	-0.02	12 (2%)	52	47	13, 51, 100, 121	2 (0%)
All	All	6471/6768 (95%)	0.19	340 (5%)	32	26	11, 53, 103, 136	35 (0%)

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	44	ASN	6.0
1	F	43	PRO	5.3
1	D	409	GLN	5.0
1	A	42	LEU	4.5
1	M	393	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	I	364	LEU	4.3
1	G	392	GLU	4.2
1	C	290	GLU	4.2
1	P	16	ARG	4.1
1	J	35	VAL	4.1
1	D	42	LEU	4.1
1	G	393	GLY	4.1
1	N	16	ARG	3.9
1	H	45	ALA	3.8
1	O	40	VAL	3.8
1	J	18	VAL	3.8
1	M	55	VAL	3.8
1	C	153	CYS	3.7
1	F	42	LEU	3.7
1	M	39	PRO	3.7
1	A	285	PHE	3.6
1	M	196	ALA	3.6
1	J	25	VAL	3.6
1	J	150	LEU	3.6
1	E	392	GLU	3.5
1	M	42	LEU	3.5
1	F	51	ARG	3.5
1	N	39	PRO	3.5
1	M	40	VAL	3.5
1	M	388	VAL	3.5
1	M	398	TYR	3.4
1	J	42	LEU	3.4
1	H	285	PHE	3.4
1	C	28	ASP	3.4
1	J	24	HIS	3.4
1	H	42	LEU	3.4
1	J	391	ASP	3.4
1	I	48	ILE	3.3
1	B	40	VAL	3.3
1	H	51	ARG	3.3
1	L	393	GLY	3.3
1	N	42	LEU	3.2
1	O	361	GLN	3.2
1	O	283	ALA	3.2
1	A	295	VAL	3.2
1	G	295	VAL	3.2
1	M	33	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	283	ALA	3.2
1	F	283	ALA	3.1
1	I	42	LEU	3.1
1	L	40	VAL	3.1
1	I	152	PRO	3.1
1	L	386	ILE	3.1
1	N	45	ALA	3.1
1	F	41	ASP	3.0
1	D	285	PHE	3.0
1	B	283	ALA	3.0
1	H	283	ALA	3.0
1	B	196	ALA	3.0
1	J	43	PRO	3.0
1	D	44	ASN	3.0
1	D	41	ASP	2.9
1	H	3	ILE	2.9
1	M	283	ALA	2.9
1	K	11	VAL	2.9
1	A	44	ASN	2.9
1	C	379	ASP	2.9
1	D	391	ASP	2.9
1	F	194	GLY	2.9
1	M	47	ALA	2.9
1	F	40	VAL	2.9
1	K	292	VAL	2.9
1	D	39	PRO	2.9
1	M	10	ASN	2.9
1	L	296	ALA	2.9
1	L	35	VAL	2.9
1	P	295	VAL	2.9
1	D	43	PRO	2.8
1	I	196	ALA	2.8
1	J	6	LEU	2.8
1	L	42	LEU	2.8
1	N	283	ALA	2.8
1	C	39	PRO	2.8
1	K	43	PRO	2.8
1	H	295	VAL	2.8
1	I	43	PRO	2.8
1	C	282	GLY	2.8
1	N	6	LEU	2.8
1	K	394	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	P	15	GLU	2.8
1	M	377	VAL	2.8
1	P	2	THR	2.8
1	P	296	ALA	2.8
1	I	12	LEU	2.7
1	D	40	VAL	2.7
1	C	3	ILE	2.7
1	K	150	LEU	2.7
1	N	149	LEU	2.7
1	L	266	ALA	2.7
1	M	25	VAL	2.7
1	L	48	ILE	2.7
1	F	44	ASN	2.7
1	F	154	SER	2.7
1	H	40	VAL	2.7
1	I	40	VAL	2.7
1	H	409	GLN	2.7
1	J	48	ILE	2.7
1	L	14	LEU	2.7
1	D	50	VAL	2.7
1	J	40	VAL	2.7
1	K	18	VAL	2.7
1	M	394	ALA	2.7
1	N	26	VAL	2.7
1	F	39	PRO	2.7
1	D	295	VAL	2.6
1	M	36	THR	2.6
1	L	400	LEU	2.6
1	A	50	VAL	2.6
1	E	283	ALA	2.6
1	N	295	VAL	2.6
1	I	289	PRO	2.6
1	M	409	GLN	2.6
1	F	290	GLU	2.6
1	C	283	ALA	2.6
1	D	45	ALA	2.6
1	F	292	VAL	2.6
1	H	2	THR	2.6
1	C	27	ILE	2.6
1	B	39	PRO	2.6
1	B	295	VAL	2.6
1	L	55	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	376	VAL	2.6
1	M	285	PHE	2.6
1	C	2	THR	2.5
1	I	22	HIS	2.5
1	N	52	GLY	2.5
1	L	50	VAL	2.5
1	I	296	ALA	2.5
1	M	45	ALA	2.5
1	O	196	ALA	2.5
1	L	36	THR	2.5
1	M	6	LEU	2.5
1	K	22	HIS	2.5
1	K	333	GLU	2.5
1	L	29	GLY	2.5
1	H	43	PRO	2.5
1	M	43	PRO	2.5
1	E	295	VAL	2.5
1	D	283	ALA	2.5
1	I	293	ALA	2.5
1	J	394	ALA	2.5
1	P	44	ASN	2.5
1	D	3	ILE	2.5
1	I	393	GLY	2.5
1	J	376	VAL	2.5
1	L	11	VAL	2.5
1	D	151	GLU	2.5
1	N	389	VAL	2.5
1	H	196	ALA	2.5
1	K	2	THR	2.4
1	A	41	ASP	2.4
1	J	152	PRO	2.4
1	J	50	VAL	2.4
1	L	394	ALA	2.4
1	F	38	ARG	2.4
1	N	48	ILE	2.4
1	K	24	HIS	2.4
1	K	289	PRO	2.4
1	G	292	VAL	2.4
1	L	6	LEU	2.4
1	L	19	LEU	2.4
1	J	22	HIS	2.4
1	A	393	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	362	GLY	2.4
1	J	7	GLN	2.4
1	I	35	VAL	2.4
1	I	195	VAL	2.4
1	M	389	VAL	2.4
1	P	18	VAL	2.4
1	J	285	PHE	2.4
1	F	278	LEU	2.4
1	I	6	LEU	2.4
1	B	2	THR	2.4
1	E	3	ILE	2.4
1	M	19	LEU	2.4
1	N	22	HIS	2.4
1	D	15	GLU	2.4
1	M	153	CYS	2.4
1	E	393	GLY	2.4
1	C	38	ARG	2.4
1	G	50	VAL	2.4
1	H	50	VAL	2.4
1	L	295	VAL	2.4
1	A	45	ALA	2.4
1	B	394	ALA	2.4
1	M	310	ALA	2.4
1	J	398	TYR	2.3
1	E	291	SER	2.3
1	A	153	CYS	2.3
1	B	155	CYS	2.3
1	L	39	PRO	2.3
1	C	52	GLY	2.3
1	J	29	GLY	2.3
1	L	317	GLY	2.3
1	A	38	ARG	2.3
1	L	18	VAL	2.3
1	J	378	LEU	2.3
1	O	42	LEU	2.3
1	J	27	ILE	2.3
1	D	2	THR	2.3
1	L	382	PRO	2.3
1	F	46	GLN	2.3
1	A	40	VAL	2.3
1	G	298	VAL	2.3
1	J	33	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	35	VAL	2.3
1	E	279	ALA	2.3
1	I	2	THR	2.3
1	I	199	THR	2.3
1	I	39	PRO	2.3
1	M	399	VAL	2.3
1	K	383	LEU	2.3
1	D	196	ALA	2.3
1	L	196	ALA	2.3
1	D	28	ASP	2.3
1	M	8	GLY	2.3
1	I	292	VAL	2.3
1	J	11	VAL	2.3
1	J	389	VAL	2.3
1	K	33	VAL	2.3
1	M	378	LEU	2.3
1	N	378	LEU	2.3
1	C	51	ARG	2.2
1	J	382	PRO	2.2
1	H	46	GLN	2.2
1	K	282	GLY	2.2
1	A	12	LEU	2.2
1	J	55	VAL	2.2
1	O	292	VAL	2.2
1	N	24	HIS	2.2
1	P	196	ALA	2.2
1	P	279	ALA	2.2
1	H	392	GLU	2.2
1	G	51	ARG	2.2
1	B	43	PRO	2.2
1	H	39	PRO	2.2
1	J	52	GLY	2.2
1	M	58	GLY	2.2
1	I	295	VAL	2.2
1	L	33	VAL	2.2
1	D	284	GLU	2.2
1	H	397	GLU	2.2
1	H	38	ARG	2.2
1	L	7	GLN	2.2
1	M	7	GLN	2.2
1	K	286	GLY	2.2
1	C	291	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	298	VAL	2.2
1	M	18	VAL	2.2
1	J	367	ILE	2.2
1	M	386	ILE	2.2
1	C	263	GLU	2.2
1	F	397	GLU	2.2
1	E	2	THR	2.2
1	H	199	THR	2.2
1	D	289	PRO	2.2
1	E	299	GLN	2.2
1	L	409	GLN	2.2
1	J	8	GLY	2.2
1	D	13	ASP	2.2
1	E	41	ASP	2.2
1	C	40	VAL	2.2
1	N	25	VAL	2.2
1	P	22	HIS	2.2
1	E	45	ALA	2.1
1	B	51	ARG	2.1
1	J	16	ARG	2.1
1	C	409	GLN	2.1
1	I	19	LEU	2.1
1	K	19	LEU	2.1
1	N	405	LEU	2.1
1	N	393	GLY	2.1
1	I	366	VAL	2.1
1	J	5	VAL	2.1
1	N	297	SER	2.1
1	M	312	ALA	2.1
1	H	290	GLU	2.1
1	N	307	GLU	2.1
1	D	51	ARG	2.1
1	M	38	ARG	2.1
1	A	43	PRO	2.1
1	I	300	GLN	2.1
1	H	282	GLY	2.1
1	M	22	HIS	2.1
1	N	28	ASP	2.1
1	B	290	GLU	2.1
1	O	2	THR	2.1
1	J	53	LYS	2.1
1	M	12	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	282	GLY	2.1
1	J	386	ILE	2.1
1	N	298	VAL	2.1
1	K	285	PHE	2.1
1	B	392	GLU	2.1
1	G	283	ALA	2.1
1	H	16	ARG	2.1
1	K	293	ALA	2.1
1	F	409	GLN	2.1
1	I	361	GLN	2.1
1	D	282	GLY	2.1
1	M	50	VAL	2.1
1	M	298	VAL	2.1
1	F	395	ARG	2.0
1	I	34	GLU	2.0
1	O	297	SER	2.0
1	L	2	THR	2.0
1	K	198	PRO	2.0
1	G	46	GLN	2.0
1	M	20	LEU	2.0
1	K	365	GLY	2.0
1	F	33	VAL	2.0
1	H	298	VAL	2.0
1	P	51	ARG	2.0
1	F	45	ALA	2.0
1	J	354	ALA	2.0
1	M	293	ALA	2.0
1	O	293	ALA	2.0
1	C	287	MET	2.0
1	M	289	PRO	2.0
1	J	347	LEU	2.0
1	P	42	LEU	2.0
1	F	22	HIS	2.0
1	H	22	HIS	2.0
1	B	298	VAL	2.0
1	D	389	VAL	2.0
1	M	195	VAL	2.0
1	N	11	VAL	2.0
1	N	33	VAL	2.0
1	N	388	VAL	2.0
1	O	298	VAL	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(Å ²)	Q<0.9
2	ZN	J	426	1/1	0.79	0.13	68,68,68,68	1
2	ZN	J	425	1/1	0.83	0.11	60,60,60,60	1
2	ZN	O	426	1/1	0.84	0.17	58,58,58,58	1
2	ZN	N	425	1/1	0.85	0.11	41,41,41,41	1
2	ZN	I	426	1/1	0.87	0.14	58,58,58,58	1
2	ZN	P	425	1/1	0.87	0.11	47,47,47,47	1
2	ZN	F	426	1/1	0.88	0.16	51,51,51,51	1
2	ZN	N	426	1/1	0.89	0.16	55,55,55,55	1
2	ZN	F	425	1/1	0.90	0.10	52,52,52,52	1
2	ZN	K	426	1/1	0.90	0.09	68,68,68,68	1
2	ZN	P	426	1/1	0.90	0.13	59,59,59,59	1
2	ZN	L	425	1/1	0.91	0.06	55,55,55,55	1
2	ZN	E	425	1/1	0.91	0.10	43,43,43,43	1
2	ZN	H	426	1/1	0.91	0.12	39,39,39,39	1
2	ZN	M	425	1/1	0.92	0.06	50,50,50,50	1
2	ZN	K	425	1/1	0.92	0.10	55,55,55,55	1
2	ZN	M	426	1/1	0.93	0.13	63,63,63,63	1
2	ZN	L	426	1/1	0.93	0.10	63,63,63,63	1
2	ZN	A	425	1/1	0.93	0.10	51,51,51,51	1
2	ZN	G	425	1/1	0.94	0.10	40,40,40,40	1
2	ZN	E	426	1/1	0.94	0.17	45,45,45,45	1
2	ZN	I	425	1/1	0.95	0.07	42,42,42,42	1
2	ZN	B	425	1/1	0.95	0.11	44,44,44,44	1
2	ZN	O	425	1/1	0.95	0.09	50,50,50,50	1
2	ZN	C	425	1/1	0.96	0.11	42,42,42,42	1
2	ZN	D	426	1/1	0.96	0.11	33,33,33,33	1
2	ZN	B	426	1/1	0.97	0.08	44,44,44,44	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	426	1/1	0.97	0.07	52,52,52,52	1
2	ZN	G	426	1/1	0.97	0.08	37,37,37,37	1
2	ZN	C	426	1/1	0.97	0.08	38,38,38,38	1
2	ZN	D	425	1/1	0.97	0.08	34,34,34,34	1
2	ZN	H	425	1/1	0.98	0.08	40,40,40,40	1

6.5 Other polymers [i](#)

There are no such residues in this entry.