



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:01 am GMT

PDB ID : 3FEQ
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

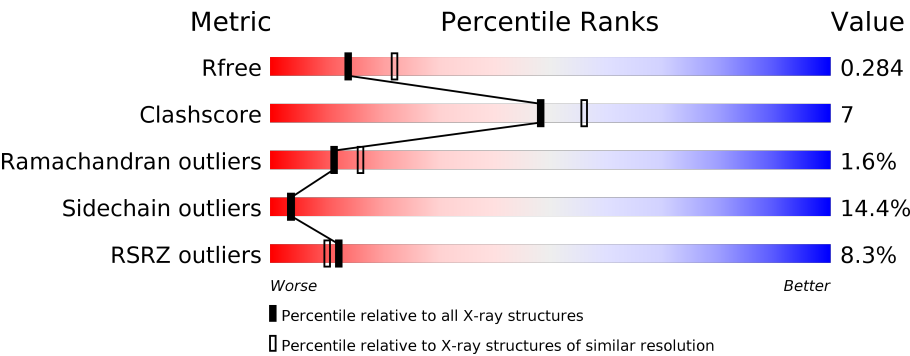
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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}	100719	1044 (2.66-2.62)
Clashscore	112137	1092 (2.66-2.62)
Ramachandran outliers	110173	1077 (2.66-2.62)
Sidechain outliers	110143	1077 (2.66-2.62)
RSRZ outliers	101464	1047 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div><div>2%</div><div><div></div><div>70%</div><div>22%</div><div>..</div></div></div>
1	B	423	<div><div>3%</div><div><div></div><div>72%</div><div>20%</div><div>..</div></div></div>
1	C	423	<div><div>4%</div><div><div></div><div>71%</div><div>22%</div><div>..</div></div></div>
1	D	423	<div><div>%</div><div><div></div><div>71%</div><div>22%</div><div>..</div></div></div>
1	E	423	<div><div>3%</div><div><div></div><div>74%</div><div>19%</div><div>..</div></div></div>
1	F	423	<div><div>3%</div><div><div></div><div>73%</div><div>18%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
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	

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
2	ZN	C	425	-	-	-	X
2	ZN	C	426	-	-	-	X
2	ZN	D	426	-	-	-	X
2	ZN	E	426	-	-	-	X
2	ZN	F	426	-	-	-	X
2	ZN	H	425	-	-	-	X
2	ZN	J	425	-	-	-	X
2	ZN	J	426	-	-	-	X
2	ZN	L	425	-	-	-	X
2	ZN	L	426	-	-	-	X
2	ZN	M	426	-	-	-	X
2	ZN	N	425	-	-	-	X
2	ZN	N	426	-	-	-	X
2	ZN	O	425	-	-	-	X
2	ZN	O	426	-	-	-	X
2	ZN	P	426	-	-	-	X

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 (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total 2	Zn 2	0	0
2	G	2	Total 2	Zn 2	0	0
2	J	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	K	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	I	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	A	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	L	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0
2	M	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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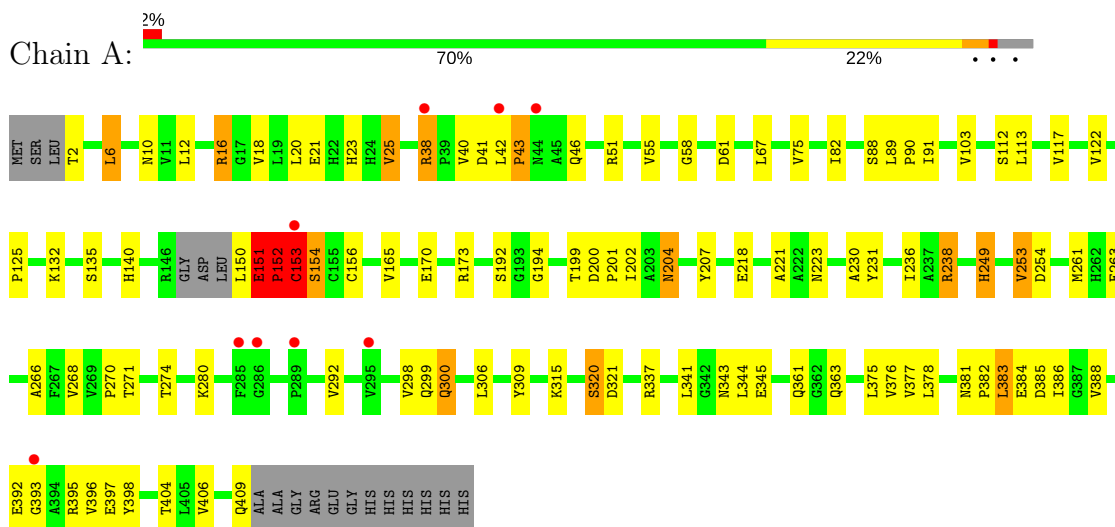
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	20	Total 20	O 20	0	0
3	E	18	Total 18	O 18	0	0
3	F	17	Total 17	O 17	0	0
3	G	16	Total 16	O 16	0	0
3	H	6	Total 6	O 6	0	0
3	O	2	Total 2	O 2	0	0
3	P	2	Total 2	O 2	0	0

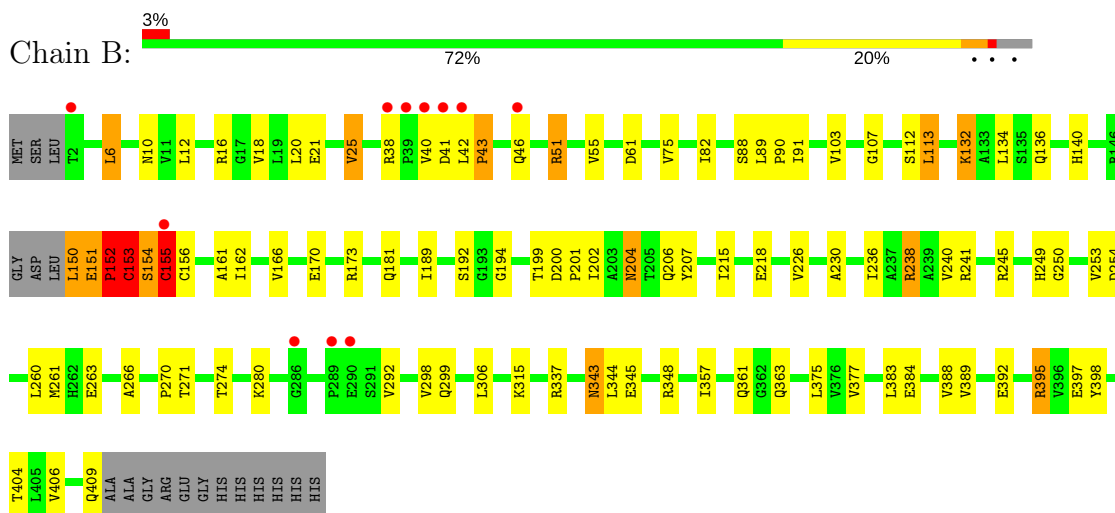
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

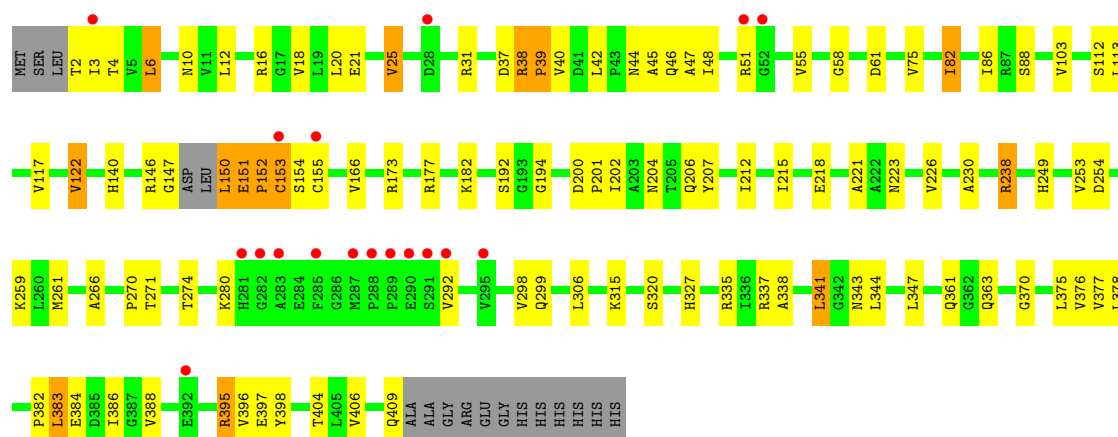


• Molecule 1: PUTATIVE AMIDOHYDROLASE

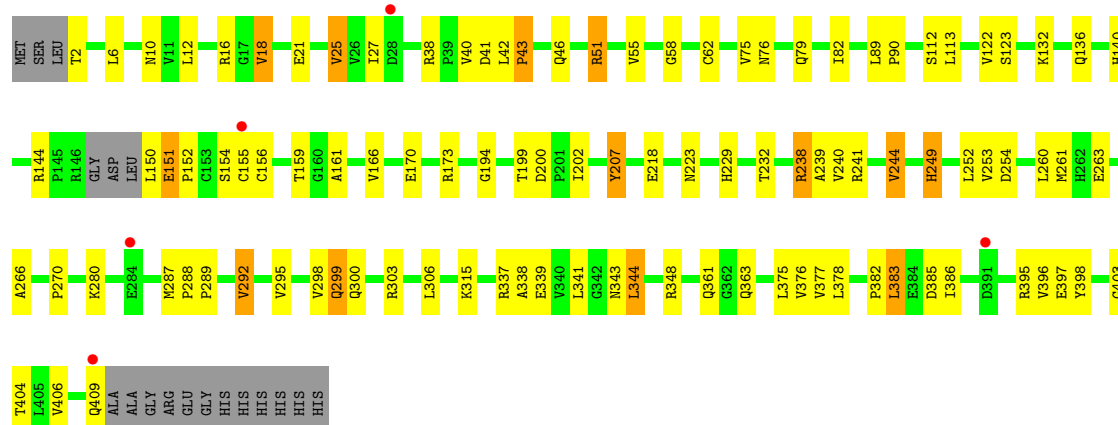


• Molecule 1: PUTATIVE AMIDOHYDROLASE

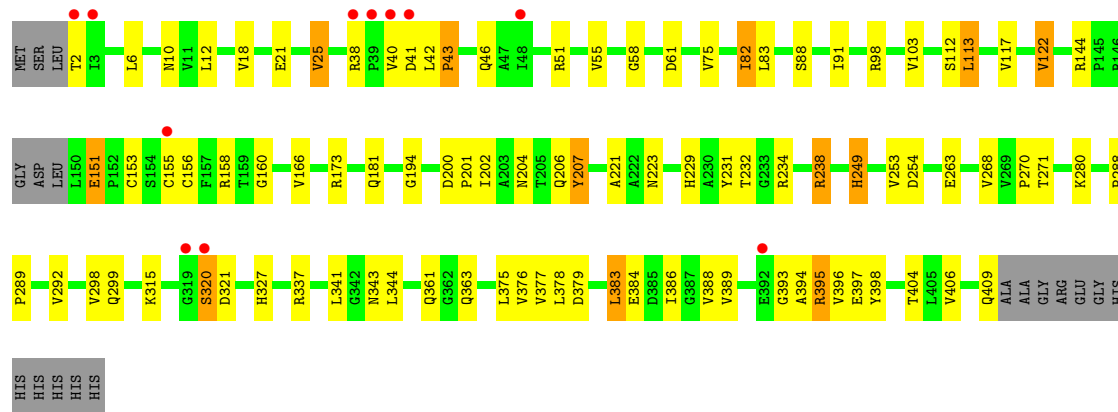
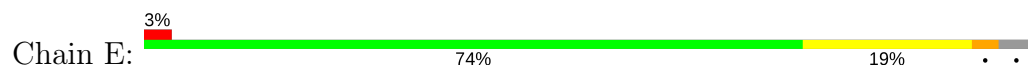




• Molecule 1: PUTATIVE AMIDOHYDROLASE

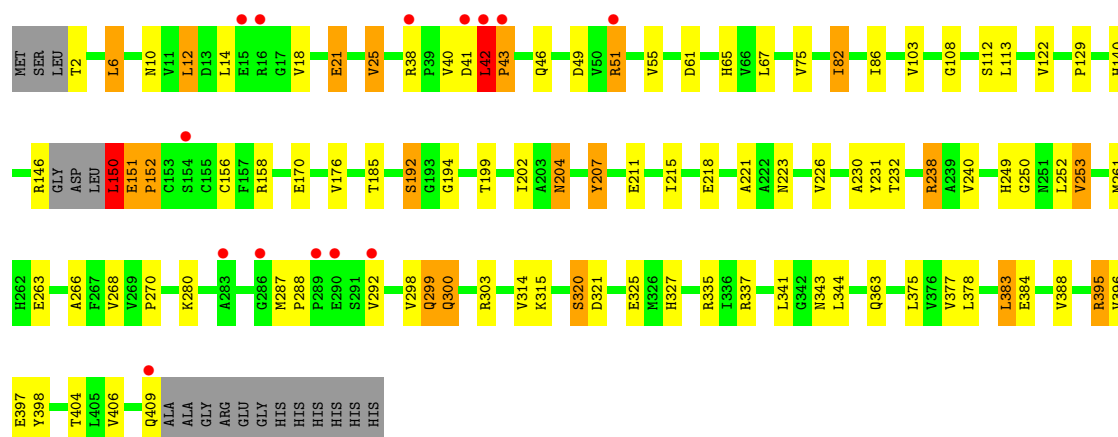


• Molecule 1: PUTATIVE AMIDOHYDROLASE

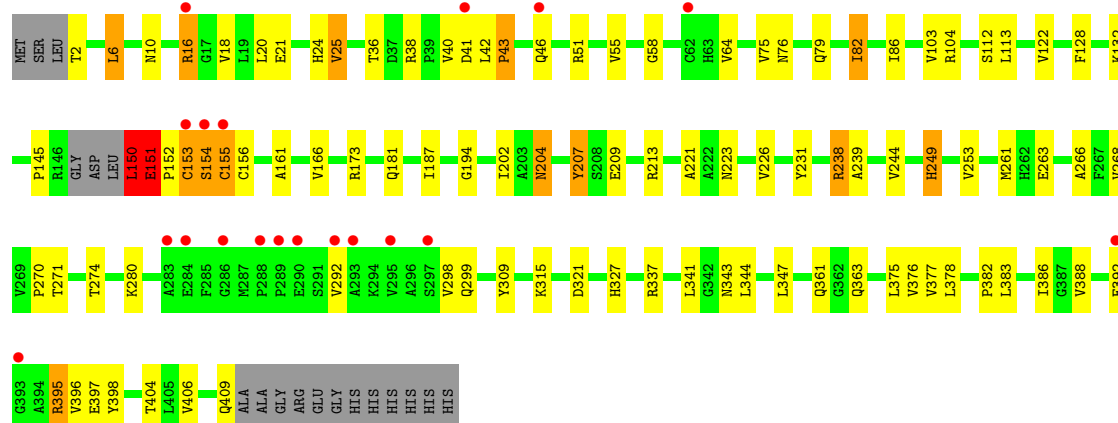
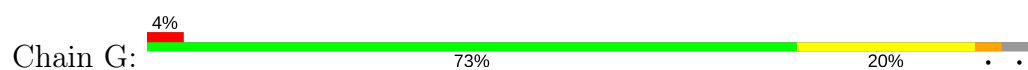


• Molecule 1: PUTATIVE AMIDOHYDROLASE

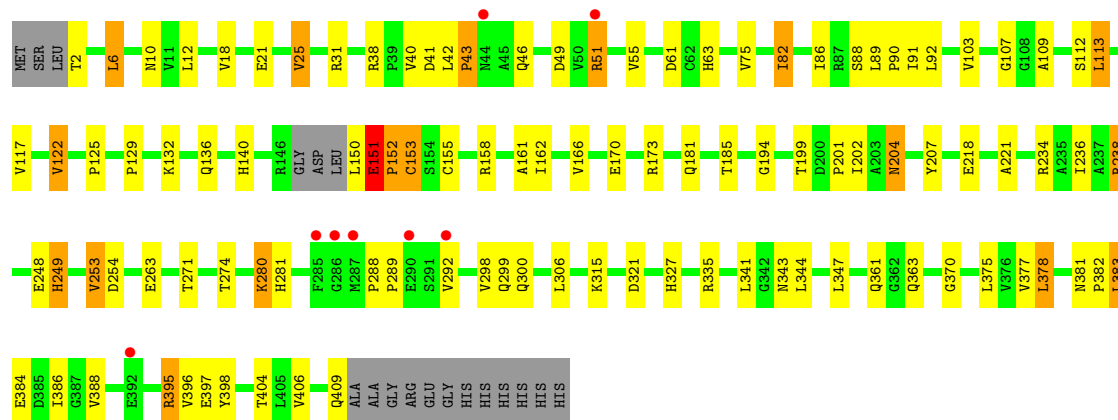




• Molecule 1: PUTATIVE AMIDOHYDROLASE

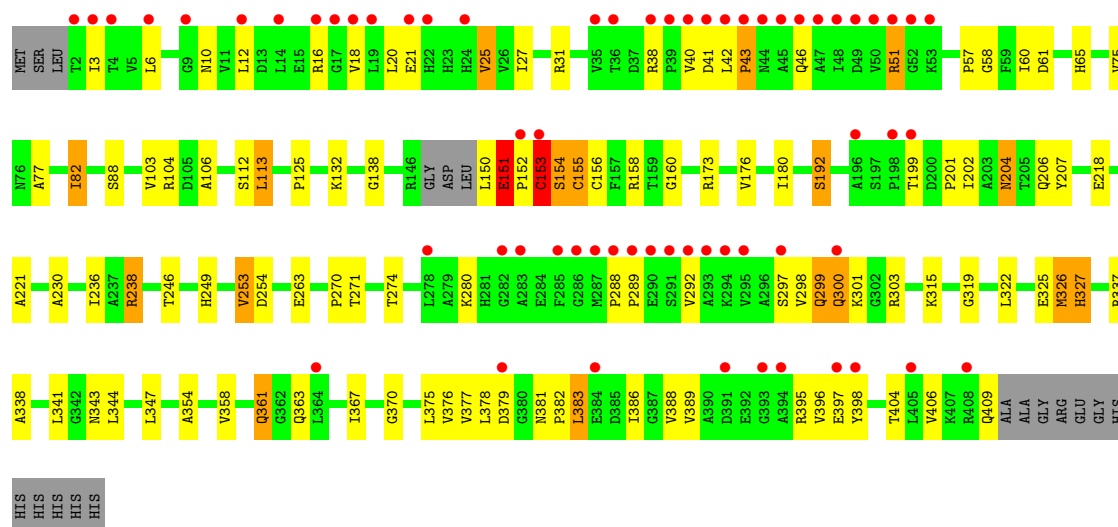


• Molecule 1: PUTATIVE AMIDOHYDROLASE

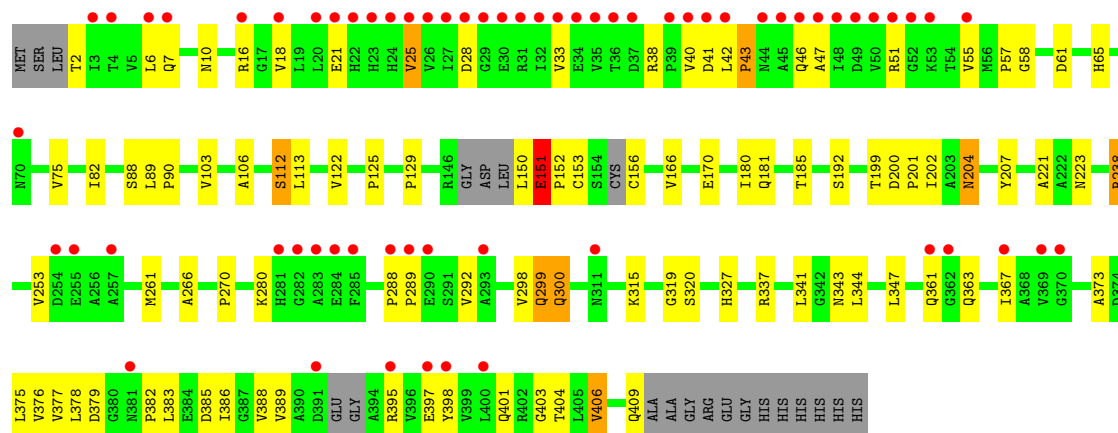


• Molecule 1: PUTATIVE AMIDOHYDROLASE

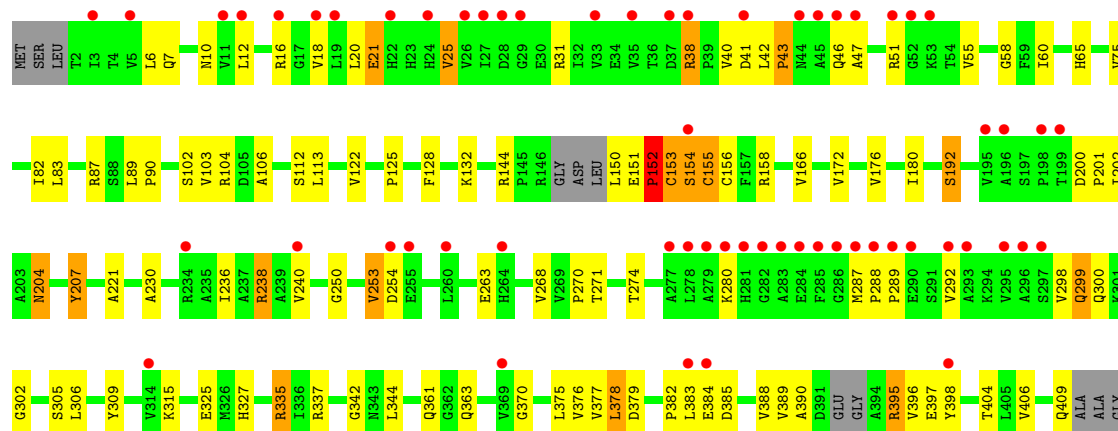




• Molecule 1: PUTATIVE AMIDOHYDROLASE

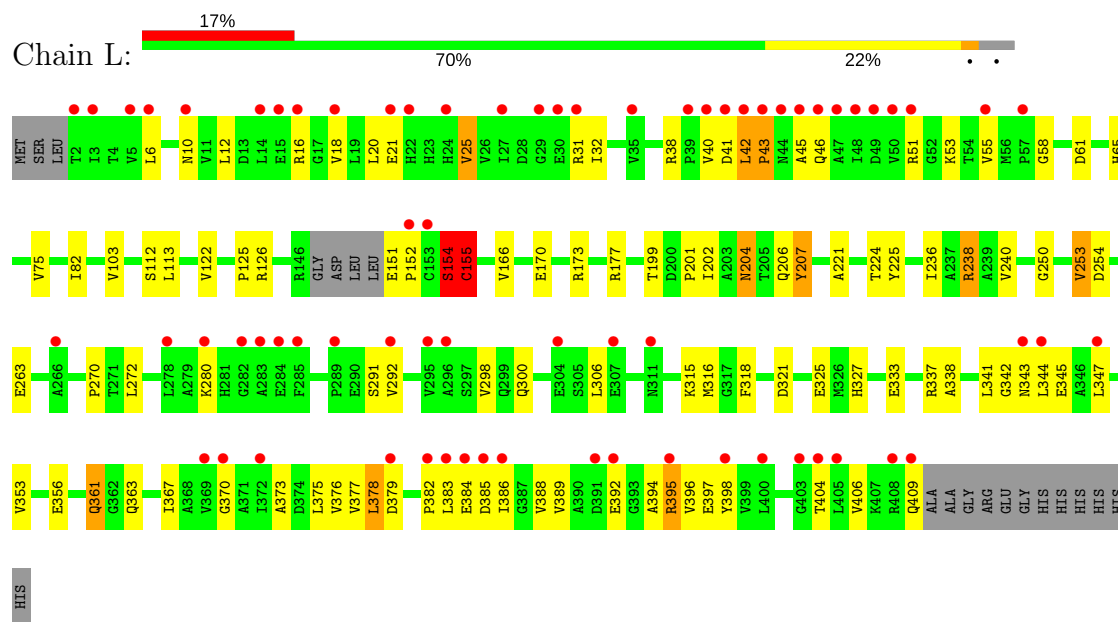


• Molecule 1: PUTATIVE AMIDOHYDROLASE

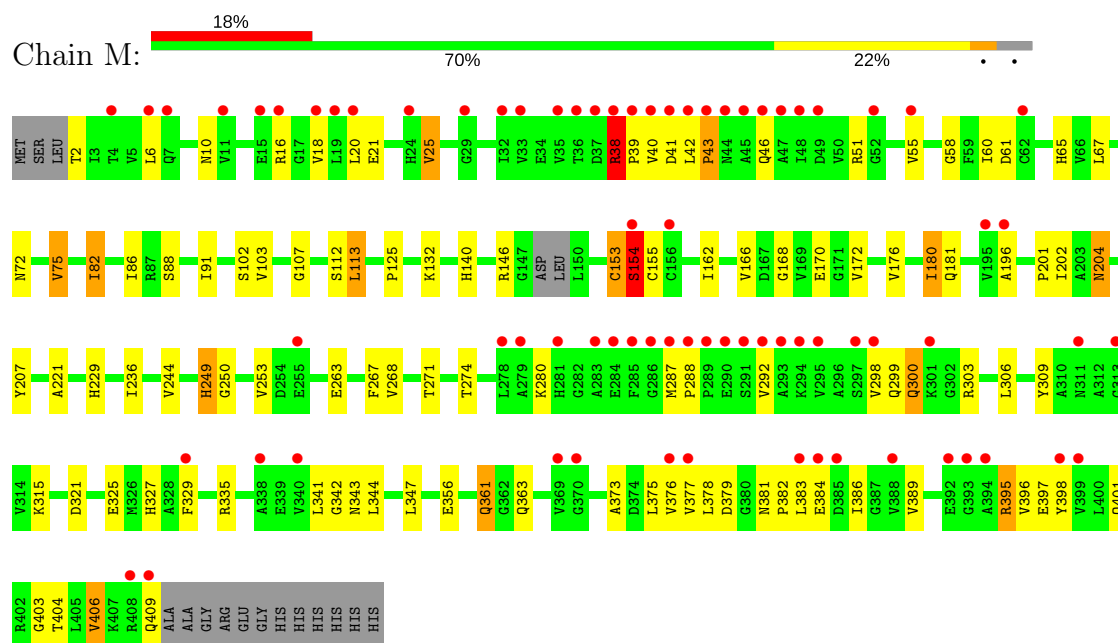


ARG
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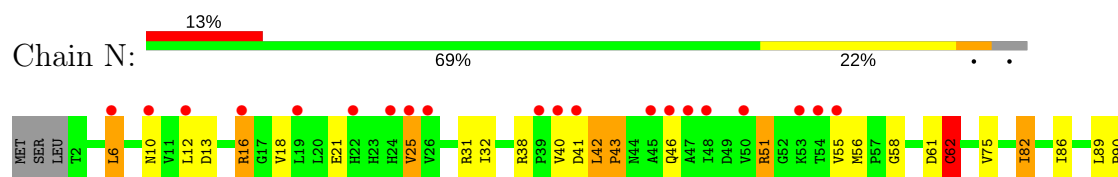
• Molecule 1: PUTATIVE AMIDOHYDROLASE



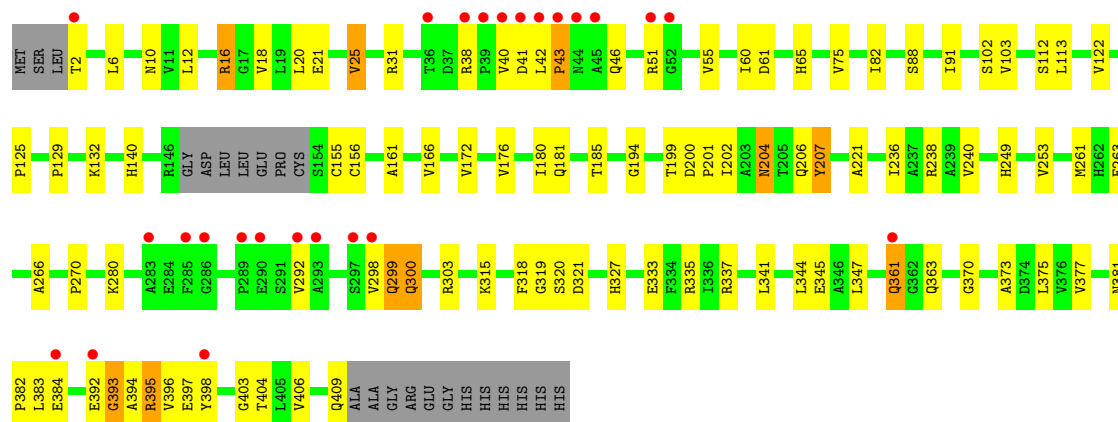
• Molecule 1: PUTATIVE AMIDOHYDROLASE



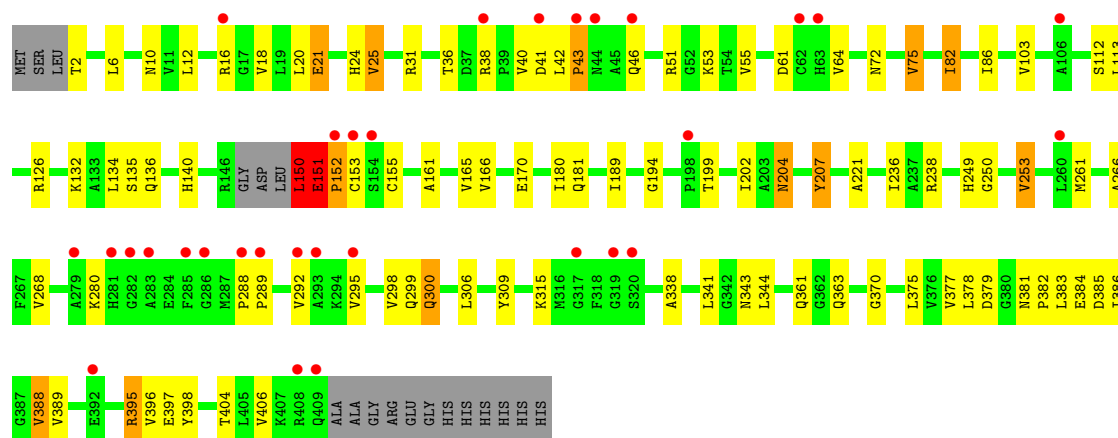
• Molecule 1: PUTATIVE AMIDOHYDROLASE



• 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 35.90 – 2.63	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-2.63) 93.4 (35.90-2.63)	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 (3.10%)	DCC
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.3	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	0.41	0/3083	0.58	2/4180 (0.0%)
1	B	0.44	0/3102	0.58	1/4205 (0.0%)
1	C	0.43	0/3074	0.55	0/4167
1	D	0.46	1/3090 (0.0%)	0.57	0/4188
1	E	0.43	0/3081	0.58	1/4177 (0.0%)
1	F	0.41	0/3065	0.59	1/4156 (0.0%)
1	G	0.41	0/3070	0.56	0/4162
1	H	0.44	0/3065	0.56	0/4156
1	I	0.46	0/3059	0.56	0/4148
1	J	0.44	0/3038	0.53	0/4117
1	K	0.44	0/3045	0.55	0/4128
1	L	0.43	0/3051	0.54	0/4137
1	M	0.43	0/3063	0.56	0/4153
1	N	0.44	1/3048 (0.0%)	0.54	0/4132
1	O	0.41	0/3028	0.54	0/4105
1	P	0.42	0/3067	0.57	0/4159
All	All	0.43	2/49029 (0.0%)	0.56	5/66470 (0.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	62	CYS	CB-SG	-6.20	1.71	1.82
1	D	62	CYS	CB-SG	-5.68	1.72	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	F	42	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	238	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	E	173	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	16	ARG	NE-CZ-NH1	-5.08	117.76	120.30

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

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Mol	Chain	Res	Type	Group
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
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	47	0
1	B	3040	0	3063	45	0
1	C	3025	0	3041	43	1
1	D	3035	0	3059	43	0
1	E	3026	0	3040	39	0
1	F	3016	0	3030	45	0
1	G	3021	0	3038	38	0
1	H	3016	0	3030	51	0
1	I	3013	0	3025	58	1
1	J	2994	0	3009	39	0
1	K	3000	0	3015	43	0
1	L	3005	0	3014	40	0
1	M	3017	0	3028	51	0
1	N	3003	0	3014	55	0
1	O	2983	0	2996	36	0
1	P	3018	0	3031	40	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	663	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 (663) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N:146:ARG:CG	1:N:147:GLY:N	2.56	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: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:M:343:ASN:HD22	1:M:386:ILE:HB	1.60	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:150:LEU:C	1:D:151:GLU:HG3	2.18	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
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: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:N:347:LEU:HD11	1:N:382:PRO:HB2	1.84	0.59
1:H:263:GLU:HB3	1:M:39:PRO:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:ARG:NH2	1:H:370:GLY:O	2.36	0.58
1:J:343:ASN:HD22	1:J:386:ILE:HB	1.68	0.58
1:B:154:SER:OG	1:B:155:CYS:N	2.36	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
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:O:41:ASP:O	1:O:43:PRO:HD3	2.04	0.57
1:J:199:THR:HG21	1:P:181:GLN:NE2	2.18	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: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:D:287:MET:HE3	1:D:292:VAL:HG22	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:61:ASP:HB3	1:H:103:VAL:HG12	1.89	0.55
1:L:154:SER:O	1:L:155:CYS:CB	2.50	0.55
1:H:263:GLU:HB3	1:M:39:PRO:CG	2.36	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
1:I:41:ASP:O	1:I:43:PRO:HD3	2.07	0.55
1:P:140:HIS:CE1	1:P:194:GLY:HA3	2.42	0.55
1:P:6:LEU:HB2	1:P:25:VAL:HG13	1.89	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:L:325:GLU:H	1:L:325:GLU:CD	2.11	0.54
1:A:199:THR:HG21	1:G:181:GLN:HE21	1.72	0.54
1:A:6:LEU:HB2	1:A:25:VAL:HG13	1.89	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: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:G:343:ASN:HB2	1:G:386:ILE:HD13	1.89	0.53
1:A:170:GLU:HA	1:A:170:GLU:OE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:224:THR:OG1	1:L:225:TYR:N	2.41	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
1:B:134:LEU:HB2	1:B:189:ILE:HG22	1.92	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: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:154:SER:O	1:N:155:CYS:CB	2.58	0.51
1:N:146:ARG:HH21	1:N:199:THR:HB	1.75	0.51
1:C:388:VAL:HA	1:C:395:ARG:HH11	1.76	0.51
1:C:82:ILE:O	1:C:86:ILE:HG12	2.10	0.51
1:K:60:ILE:HG12	1:K:102:SER:HB2	1.92	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:347:LEU:HD11	1:L:382:PRO:HB2	1.93	0.51
1:L:41:ASP:O	1:L:43:PRO:HD3	2.10	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:C:223:ASN:ND2	1:F:204:ASN:HB3	2.27	0.50
1:B:181:GLN:HE21	1:D:199:THR:HG21	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:146:ARG:HG2	1:N:147:GLY:N	2.26	0.50
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:HA	1:M:170:GLU:OE2	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: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:299:GLN:HG3	1:I:300:GLN:HE21	1.78	0.49
1:I:60:ILE:HB	1:I:354:ALA:HB1	1.95	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:A:61:ASP:OD2	1:A:320[A]:SER:OG	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:ARG:HH21	1:F:199:THR:HB	1.78	0.48
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: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:P:343:ASN:HB2	1:P:386:ILE:HD13	1.96	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: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:P:204:ASN:HD22	1:P:204:ASN:C	2.17	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: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
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:C:47:ALA:C	1:C:48:ILE:HG13	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:151:GLU:HA	1:A:151:GLU:OE1	2.14	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:O:172:VAL:O	1:O:176:VAL:HG23	2.15	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:D:51:ARG:HD2	1:D:51:ARG:O	2.15	0.46
1:H:170:GLU:HA	1:H:170:GLU:OE2	2.14	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:325:GLU:CD	1:M:325:GLU:H	2.18	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:HD22	1:C:44:ASN:H	1.62	0.46
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:HA	1:F:170:GLU:OE2	2.16	0.46
1:K:65:HIS:CE1	1:K:106:ALA:HB3	2.51	0.46
1:K:7:GLN:NE2	1:K:47:ALA:HB1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:393:GLY:O	1:E:395:ARG:N	2.48	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:N:393:GLY:C	1:N:395:ARG:H	2.18	0.45
1:O:10:ASN:HD22	1:O:21:GLU:HA	1.82	0.45
1:P:236:ILE:HG21	1:P:261:MET:CE	2.47	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HB3	1:H:335:ARG:NH1	2.31	0.44
1:K:299:GLN:HG3	1:K:300:GLN:HE21	1.82	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:I:361:GLN:CD	1:I:361:GLN:H	2.21	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:381:ASN:HA	1:I:382:PRO:HD2	1.90	0.44
1:I:378:LEU:HD21	1:I:389:VAL:HG22	1.99	0.44
1:N:56:MET:HA	1:N:367:ILE:HD11	1.98	0.44
1:P:135:SER:O	1:P:165:VAL:HA	2.18	0.44
1:H:383:LEU:HA	1:H:383:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ASN:HD22	1:B:21:GLU:HA	1.83	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:F:325:GLU:H	1:F:325:GLU:CD	2.20	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:I:199:THR:HG21	1:O:181:GLN:NE2	2.33	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:172:VAL:O	1:M:176:VAL:HG23	2.18	0.43
1:M:65:HIS:CD2	1:M:321:ASP:OD1	2.71	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:383:LEU:HA	1:E:383:LEU:HD12	1.84	0.43
1:E:61:ASP:OD2	1:E:320:SER:OG	2.31	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:B:173:ARG:HG2	1:B:218:GLU:CG	2.49	0.43
1:D:299:GLN:HG3	1:D:300:GLN:HE21	1.83	0.43
1:D:89:LEU:HD11	1:G:86:ILE:HD12	1.99	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:D:288:PRO:HA	1:D:289:PRO:HD3	1.77	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:58:GLY:HA2	1:G:376:VAL:HG23	2.01	0.43
1:G:378:LEU:HA	1:G:378:LEU:HD12	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:H:204:ASN:HD22	1:H:204:ASN:C	2.23	0.43
1:I:158:ARG:HG2	1:I:158:ARG:H	1.62	0.43
1:I:82:ILE:HD12	1:J:112:SER:HB2	1.99	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
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:154:SER:O	1:I:155:CYS:HB2	2.19	0.42
1:I:57:PRO:HG3	1:I:367:ILE:HG13	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:383:LEU:HA	1:I:383:LEU:HD12	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:206:GLN:O	1:B:207:TYR:HB2	2.19	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:HA	1:P:170:GLU:OE2	2.19	0.42
1:B:170:GLU:OE2	1:B:170:GLU:HA	2.20	0.42
1:B:51:ARG:O	1:B:51:ARG:HD2	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:G:145:PRO:HG2	1:G:150:LEU:HD23	2.01	0.42
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:I:325:GLU:C	1:I:327:HIS:H	2.23	0.42
1:D:338:ALA:HB1	1:D:343:ASN:HB3	2.01	0.41
1:H:132:LYS:HE3	1:H:161:ALA:O	2.20	0.41
1:H:49:ASP:OD1	1:H:51:ARG:NH1	2.53	0.41
1:I:176:VAL:CG1	1:I:218:GLU:HB3	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:151:GLU:N	1:F:151:GLU:OE1	2.51	0.41
1:F:158:ARG:HG2	1:F:158:ARG:H	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
1:F:250:GLY:O	1:F:253:VAL:HG22	2.20	0.41
1:H:378:LEU:HD12	1:H:378:LEU:HA	1.79	0.41
1:I:113:LEU:HA	1:I:113:LEU:HD23	1.90	0.41
1:H:263:GLU:OE2	1:M:39:PRO:HD2	2.20	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:192:SER:HB3	1:K:230:ALA:HA	2.03	0.41
1:K:89:LEU:HA	1:K:89:LEU:HD23	1.83	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:K:325:GLU:CD	1:K:325:GLU:H	2.24	0.41
1:P:150:LEU:O	1:P:151:GLU:HB2	2.21	0.41
1:E:113:LEU:HA	1:E:113:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:C:383:LEU:HD12	1.80	0.41
1:E:82:ILE:HG13	1:E:83:LEU:N	2.35	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:N:32:ILE:HD13	1:N:367:ILE:HG23	2.03	0.41
1:G:76:ASN:O	1:G:79:GLN:HG2	2.20	0.41
1:I:61:ASP:OD1	1:I:319:GLY:HA2	2.21	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:K:200:ASP:HA	1:K:201:PRO:HD2	1.85	0.41
1:K:83:LEU:HD13	1:K:87:ARG:NH1	2.36	0.41
1:M:140:HIS:HE1	1:M:196:ALA:H	1.69	0.41
1:A:200:ASP:HA	1:A:201:PRO:HD2	1.94	0.40
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: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:M:113:LEU:HD23	1:M:113:LEU:HA	1.75	0.40
1:M:107:GLY:O	1:M:162:ILE:HD12	2.21	0.40
1:D:383:LEU:HD12	1:D:383:LEU:HA	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:HD23	1:H:113:LEU:HA	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: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:302:GLY:O	1:K:305:SER:OG	2.38	0.40
1:K:38:ARG:HA	1:K:38:ARG:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:200:ASP:HA	1:B:201:PRO:HD2	1.94	0.40
1:B:89:LEU:HB2	1:B:90:PRO:HD3	2.03	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: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 symmetry 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%)	11	15
1	B	407/423 (96%)	384 (94%)	16 (4%)	7 (2%)	11	15
1	C	404/423 (96%)	380 (94%)	18 (4%)	6 (2%)	12	17
1	D	405/423 (96%)	383 (95%)	17 (4%)	5 (1%)	15	22
1	E	405/423 (96%)	378 (93%)	23 (6%)	4 (1%)	18	27
1	F	403/423 (95%)	379 (94%)	19 (5%)	5 (1%)	15	22
1	G	403/423 (95%)	380 (94%)	18 (4%)	5 (1%)	15	22
1	H	403/423 (95%)	374 (93%)	21 (5%)	8 (2%)	9	12
1	I	402/423 (95%)	374 (93%)	20 (5%)	8 (2%)	9	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	395/423 (93%)	368 (93%)	22 (6%)	5 (1%)	14	20
1	K	398/423 (94%)	369 (93%)	22 (6%)	7 (2%)	10	14
1	L	401/423 (95%)	371 (92%)	21 (5%)	9 (2%)	8	11
1	M	403/423 (95%)	378 (94%)	17 (4%)	8 (2%)	9	12
1	N	401/423 (95%)	367 (92%)	28 (7%)	6 (2%)	12	17
1	O	398/423 (94%)	373 (94%)	18 (4%)	7 (2%)	10	14
1	P	403/423 (95%)	380 (94%)	17 (4%)	6 (2%)	12	17
All	All	6436/6768 (95%)	6023 (94%)	310 (5%)	103 (2%)	11	16

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	268 (84%)	49 (16%)	3	3
1	B	319/326 (98%)	272 (85%)	47 (15%)	3	3
1	C	315/326 (97%)	267 (85%)	48 (15%)	3	3
1	D	317/326 (97%)	270 (85%)	47 (15%)	3	3
1	E	316/326 (97%)	272 (86%)	44 (14%)	4	4
1	F	315/326 (97%)	266 (84%)	49 (16%)	3	3
1	G	315/326 (97%)	272 (86%)	43 (14%)	4	5
1	H	315/326 (97%)	271 (86%)	44 (14%)	4	4
1	I	314/326 (96%)	270 (86%)	44 (14%)	4	4
1	J	312/326 (96%)	272 (87%)	40 (13%)	5	6
1	K	313/326 (96%)	265 (85%)	48 (15%)	3	3
1	L	313/326 (96%)	268 (86%)	45 (14%)	4	4
1	M	314/326 (96%)	269 (86%)	45 (14%)	4	4
1	N	312/326 (96%)	265 (85%)	47 (15%)	3	3
1	O	310/326 (95%)	266 (86%)	44 (14%)	4	4
1	P	315/326 (97%)	274 (87%)	41 (13%)	5	6
All	All	5032/5216 (96%)	4307 (86%)	725 (14%)	4	4

All (725) 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	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	132	LYS

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Mol	Chain	Res	Type
1	A	151	GLU
1	A	153	CYS
1	A	154	SER
1	A	156	CYS
1	A	202	ILE
1	A	204	ASN
1	A	238	ARG
1	A	253	VAL
1	A	254	ASP
1	A	263	GLU
1	A	280	LYS
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	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	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	25	VAL
1	B	40	VAL
1	B	42	LEU
1	B	46	GLN
1	B	51	ARG
1	B	55	VAL

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Mol	Chain	Res	Type
1	B	75	VAL
1	B	82	ILE
1	B	112	SER
1	B	113	LEU
1	B	132	LYS
1	B	150	LEU
1	B	152	PRO
1	B	153	CYS
1	B	155	CYS
1	B	156	CYS
1	B	166	VAL
1	B	202	ILE
1	B	204	ASN
1	B	238	ARG
1	B	253	VAL
1	B	254	ASP
1	B	263	GLU
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	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	383	LEU
1	B	384	GLU
1	B	389	VAL
1	B	392	GLU
1	B	395	ARG
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
1	C	25	VAL

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Mol	Chain	Res	Type
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	88	SER
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	200	ASP
1	C	202	ILE
1	C	238	ARG
1	C	253	VAL
1	C	254	ASP
1	C	259	LYS
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	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
1	C	384	GLU
1	C	395	ARG
1	C	396	VAL
1	C	397	GLU
1	C	404	THR

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Mol	Chain	Res	Type
1	C	406	VAL
1	C	409	GLN
1	D	12	LEU
1	D	18	VAL
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	122	VAL
1	D	123	SER
1	D	136	GLN
1	D	151	GLU
1	D	155	CYS
1	D	156	CYS
1	D	159	THR
1	D	166	VAL
1	D	200	ASP
1	D	202	ILE
1	D	238	ARG
1	D	244	VAL
1	D	253	VAL
1	D	254	ASP
1	D	263	GLU
1	D	280	LYS
1	D	292	VAL
1	D	298	VAL
1	D	299	GLN
1	D	306	LEU
1	D	315	LYS
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

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Mol	Chain	Res	Type
1	D	383	LEU
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	12	LEU
1	E	18	VAL
1	E	25	VAL
1	E	40	VAL
1	E	42	LEU
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	122	VAL
1	E	151	GLU
1	E	155	CYS
1	E	156	CYS
1	E	158	ARG
1	E	166	VAL
1	E	202	ILE
1	E	238	ARG
1	E	253	VAL
1	E	254	ASP
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	327	HIS
1	E	341	LEU
1	E	344	LEU
1	E	361	GLN
1	E	363	GLN

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Mol	Chain	Res	Type
1	E	375	LEU
1	E	383	LEU
1	E	384	GLU
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	38	ARG
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
1	F	113	LEU
1	F	122	VAL
1	F	150	LEU
1	F	151	GLU
1	F	156	CYS
1	F	192	SER
1	F	202	ILE
1	F	204	ASN
1	F	238	ARG
1	F	253	VAL
1	F	263	GLU
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

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Mol	Chain	Res	Type
1	F	327	HIS
1	F	335	ARG
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	6	LEU
1	G	16	ARG
1	G	18	VAL
1	G	25	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	202	ILE
1	G	204	ASN
1	G	238	ARG
1	G	253	VAL
1	G	263	GLU
1	G	280	LYS
1	G	292	VAL

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Mol	Chain	Res	Type
1	G	298	VAL
1	G	299	GLN
1	G	315	LYS
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	383	LEU
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	6	LEU
1	H	12	LEU
1	H	18	VAL
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	122	VAL
1	H	136	GLN
1	H	151	GLU
1	H	158	ARG
1	H	166	VAL
1	H	202	ILE
1	H	204	ASN
1	H	238	ARG
1	H	253	VAL
1	H	254	ASP
1	H	280	LYS
1	H	292	VAL

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Mol	Chain	Res	Type
1	H	298	VAL
1	H	299	GLN
1	H	306	LEU
1	H	315	LYS
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	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	25	VAL
1	I	40	VAL
1	I	42	LEU
1	I	46	GLN
1	I	51	ARG
1	I	75	VAL
1	I	82	ILE
1	I	88	SER
1	I	112	SER
1	I	113	LEU
1	I	132	LYS
1	I	150	LEU
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
1	I	204	ASN
1	I	238	ARG

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Mol	Chain	Res	Type
1	I	246	THR
1	I	253	VAL
1	I	254	ASP
1	I	263	GLU
1	I	280	LYS
1	I	292	VAL
1	I	298	VAL
1	I	299	GLN
1	I	315	LYS
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	383	LEU
1	I	396	VAL
1	I	397	GLU
1	I	404	THR
1	I	406	VAL
1	I	409	GLN
1	J	16	ARG
1	J	18	VAL
1	J	25	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	88	SER
1	J	112	SER
1	J	113	LEU
1	J	122	VAL
1	J	151	GLU
1	J	156	CYS
1	J	166	VAL
1	J	180	ILE
1	J	192	SER
1	J	202	ILE
1	J	204	ASN

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Mol	Chain	Res	Type
1	J	238	ARG
1	J	253	VAL
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	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	397	GLU
1	J	404	THR
1	J	406	VAL
1	J	409	GLN
1	K	12	LEU
1	K	18	VAL
1	K	21	GLU
1	K	25	VAL
1	K	40	VAL
1	K	42	LEU
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	158	ARG
1	K	166	VAL
1	K	180	ILE
1	K	192	SER
1	K	202	ILE
1	K	204	ASN

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Mol	Chain	Res	Type
1	K	238	ARG
1	K	253	VAL
1	K	254	ASP
1	K	263	GLU
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	327	HIS
1	K	335	ARG
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	395	ARG
1	K	396	VAL
1	K	397	GLU
1	K	404	THR
1	K	406	VAL
1	K	409	GLN
1	L	12	LEU
1	L	18	VAL
1	L	25	VAL
1	L	40	VAL
1	L	42	LEU
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

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Mol	Chain	Res	Type
1	L	202	ILE
1	L	204	ASN
1	L	238	ARG
1	L	253	VAL
1	L	254	ASP
1	L	263	GLU
1	L	280	LYS
1	L	291	SER
1	L	292	VAL
1	L	298	VAL
1	L	315	LYS
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
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	18	VAL
1	M	25	VAL
1	M	38	ARG
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	132	LYS

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Mol	Chain	Res	Type
1	M	153	CYS
1	M	154	SER
1	M	155	CYS
1	M	166	VAL
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	280	LYS
1	M	292	VAL
1	M	298	VAL
1	M	303	ARG
1	M	306	LEU
1	M	315	LYS
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	16	ARG
1	N	18	VAL
1	N	25	VAL
1	N	40	VAL
1	N	42	LEU
1	N	46	GLN
1	N	51	ARG
1	N	55	VAL
1	N	62	CYS

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Mol	Chain	Res	Type
1	N	75	VAL
1	N	82	ILE
1	N	112	SER
1	N	132	LYS
1	N	135	SER
1	N	149	LEU
1	N	156	CYS
1	N	166	VAL
1	N	173	ARG
1	N	180	ILE
1	N	202	ILE
1	N	204	ASN
1	N	238	ARG
1	N	253	VAL
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	315	LYS
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	392	GLU
1	N	395	ARG
1	N	397	GLU
1	N	404	THR
1	N	406	VAL
1	N	409	GLN
1	O	12	LEU
1	O	16	ARG
1	O	18	VAL
1	O	25	VAL
1	O	40	VAL
1	O	42	LEU

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Mol	Chain	Res	Type
1	O	46	GLN
1	O	51	ARG
1	O	55	VAL
1	O	75	VAL
1	O	82	ILE
1	O	112	SER
1	O	113	LEU
1	O	122	VAL
1	O	155	CYS
1	O	156	CYS
1	O	166	VAL
1	O	180	ILE
1	O	202	ILE
1	O	204	ASN
1	O	238	ARG
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	327	HIS
1	O	341	LEU
1	O	344	LEU
1	O	345	GLU
1	O	361	GLN
1	O	363	GLN
1	O	375	LEU
1	O	383	LEU
1	O	384	GLU
1	O	395	ARG
1	O	396	VAL
1	O	397	GLU
1	O	404	THR
1	O	406	VAL
1	O	409	GLN
1	P	12	LEU
1	P	18	VAL
1	P	21	GLU
1	P	25	VAL

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Mol	Chain	Res	Type
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	126	ARG
1	P	136	GLN
1	P	150	LEU
1	P	155	CYS
1	P	166	VAL
1	P	180	ILE
1	P	202	ILE
1	P	204	ASN
1	P	253	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	341	LEU
1	P	344	LEU
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN

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Mol	Chain	Res	Type
1	A	24	HIS
1	A	299	GLN
1	A	300	GLN
1	B	10	ASN
1	B	46	GLN
1	B	299	GLN
1	B	300	GLN
1	B	401	GLN
1	C	10	ASN
1	C	44	ASN
1	C	299	GLN
1	C	300	GLN
1	C	361	GLN
1	D	10	ASN
1	D	46	GLN
1	D	299	GLN
1	D	300	GLN
1	D	401	GLN
1	E	10	ASN
1	E	299	GLN
1	E	300	GLN
1	E	361	GLN
1	F	10	ASN
1	F	299	GLN
1	F	300	GLN
1	F	401	GLN
1	G	10	ASN
1	G	299	GLN
1	G	300	GLN
1	H	10	ASN
1	H	299	GLN
1	H	300	GLN
1	H	361	GLN
1	I	10	ASN
1	I	204	ASN
1	I	299	GLN
1	I	300	GLN
1	J	10	ASN
1	J	65	HIS
1	J	299	GLN
1	J	300	GLN
1	K	10	ASN

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Mol	Chain	Res	Type
1	K	223	ASN
1	K	299	GLN
1	K	300	GLN
1	K	361	GLN
1	L	10	ASN
1	L	24	HIS
1	L	204	ASN
1	L	299	GLN
1	L	300	GLN
1	L	361	GLN
1	M	10	ASN
1	M	204	ASN
1	M	299	GLN
1	M	300	GLN
1	M	361	GLN
1	N	10	ASN
1	N	204	ASN
1	N	299	GLN
1	N	300	GLN
1	N	361	GLN
1	O	10	ASN
1	O	204	ASN
1	O	299	GLN
1	O	300	GLN
1	P	10	ASN
1	P	204	ASN
1	P	299	GLN
1	P	300	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	405/423 (95%)	-0.11	9 (2%) 62 58	16, 50, 100, 117	0
1	B	405/423 (95%)	-0.03	11 (2%) 55 50	11, 48, 102, 119	0
1	C	406/423 (95%)	0.04	18 (4%) 35 31	14, 49, 104, 118	0
1	D	405/423 (95%)	-0.01	5 (1%) 79 77	14, 44, 98, 116	0
1	E	405/423 (95%)	0.04	11 (2%) 55 50	14, 47, 102, 119	0
1	F	405/423 (95%)	0.03	14 (3%) 44 40	15, 49, 99, 119	0
1	G	405/423 (95%)	0.09	19 (4%) 32 28	18, 50, 103, 136	0
1	H	405/423 (95%)	-0.01	8 (1%) 65 61	12, 46, 100, 119	0
1	I	405/423 (95%)	0.62	63 (15%) 2 1	28, 58, 106, 123	0
1	J	402/423 (95%)	0.59	64 (15%) 2 1	27, 60, 103, 121	0
1	K	403/423 (95%)	0.62	60 (14%) 3 1	25, 59, 103, 119	0
1	L	404/423 (95%)	0.68	70 (17%) 2 1	22, 61, 106, 133	0
1	M	406/423 (95%)	0.81	75 (18%) 1 1	23, 60, 107, 130	0
1	N	404/423 (95%)	0.51	53 (13%) 4 2	21, 58, 106, 121	0
1	O	401/423 (94%)	0.02	25 (6%) 21 19	22, 53, 103, 121	0
1	P	405/423 (95%)	0.19	31 (7%) 14 11	13, 51, 100, 121	0
All	All	6471/6768 (95%)	0.25	536 (8%) 12 10	11, 53, 103, 136	0

All (536) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	290	GLU	8.5
1	M	393	GLY	8.2
1	J	18	VAL	7.9
1	M	398	TYR	7.3
1	J	6	LEU	7.1

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Mol	Chain	Res	Type	RSRZ
1	G	392	GLU	6.9
1	I	152	PRO	6.7
1	I	40	VAL	6.6
1	K	18	VAL	6.6
1	O	289	PRO	6.6
1	M	392	GLU	6.5
1	M	39	PRO	6.4
1	M	297	SER	6.4
1	M	45	ALA	6.3
1	J	42	LEU	6.2
1	F	43	PRO	6.2
1	I	12	LEU	6.1
1	O	44	ASN	6.0
1	I	38	ARG	6.0
1	M	288	PRO	6.0
1	J	35	VAL	5.9
1	M	40	VAL	5.9
1	J	283	ALA	5.9
1	M	47	ALA	5.9
1	M	285	PHE	5.8
1	M	289	PRO	5.8
1	I	41	ASP	5.7
1	B	40	VAL	5.7
1	K	286	GLY	5.7
1	M	409	GLN	5.7
1	P	44	ASN	5.6
1	J	285	PHE	5.6
1	J	24	HIS	5.6
1	I	48	ILE	5.5
1	I	286	GLY	5.5
1	P	289	PRO	5.4
1	K	35	VAL	5.3
1	L	44	ASN	5.2
1	M	196	ALA	5.2
1	M	43	PRO	5.2
1	I	289	PRO	5.2
1	J	46	GLN	5.1
1	N	16	ARG	5.1
1	H	285	PHE	5.0
1	I	39	PRO	5.0
1	J	27	ILE	5.0
1	J	290	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	J	25	VAL	5.0
1	L	369	VAL	5.0
1	G	283	ALA	4.9
1	K	281	HIS	4.9
1	K	288	PRO	4.8
1	N	289	PRO	4.7
1	L	15	GLU	4.7
1	M	298	VAL	4.7
1	M	33	VAL	4.7
1	C	292	VAL	4.7
1	K	285	PHE	4.7
1	C	288	PRO	4.6
1	C	283	ALA	4.6
1	J	39	PRO	4.6
1	N	45	ALA	4.6
1	M	292	VAL	4.6
1	K	24	HIS	4.5
1	L	386	ILE	4.5
1	M	44	ASN	4.5
1	I	288	PRO	4.5
1	I	18	VAL	4.5
1	J	52	GLY	4.5
1	M	291	SER	4.5
1	L	383	LEU	4.5
1	F	290	GLU	4.5
1	L	18	VAL	4.5
1	G	393	GLY	4.5
1	M	293	ALA	4.4
1	P	283	ALA	4.4
1	J	40	VAL	4.4
1	M	290	GLU	4.4
1	M	384	GLU	4.4
1	I	293	ALA	4.4
1	N	46	GLN	4.4
1	I	2	THR	4.4
1	F	286	GLY	4.3
1	I	285	PHE	4.3
1	I	295	VAL	4.3
1	O	45	ALA	4.3
1	J	41	ASP	4.3
1	K	196	ALA	4.3
1	I	35	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	M	295	VAL	4.3
1	M	48	ILE	4.2
1	K	198	PRO	4.2
1	E	41	ASP	4.2
1	L	2	THR	4.2
1	K	282	GLY	4.2
1	J	289	PRO	4.2
1	K	290	GLU	4.1
1	L	296	ALA	4.1
1	A	44	ASN	4.1
1	B	41	ASP	4.1
1	I	50	VAL	4.1
1	I	364	LEU	4.1
1	L	400	LEU	4.1
1	K	295	VAL	4.1
1	C	289	PRO	4.1
1	O	286	GLY	4.1
1	J	45	ALA	4.1
1	M	49	ASP	4.1
1	N	383	LEU	4.1
1	L	284	GLU	4.0
1	L	29	GLY	4.0
1	K	287	MET	4.0
1	O	41	ASP	4.0
1	O	293	ALA	4.0
1	I	22	HIS	4.0
1	I	408	ARG	4.0
1	L	35	VAL	4.0
1	N	379	ASP	3.9
1	N	389	VAL	3.9
1	O	297	SER	3.9
1	K	398	TYR	3.9
1	N	286	GLY	3.9
1	I	6	LEU	3.9
1	M	370	GLY	3.9
1	M	7	GLN	3.9
1	N	6	LEU	3.9
1	N	395	ARG	3.9
1	L	16	ARG	3.8
1	L	384	GLU	3.8
1	F	283	ALA	3.8
1	N	385	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	N	408	ARG	3.8
1	N	40	VAL	3.8
1	C	153	CYS	3.8
1	J	48	ILE	3.8
1	L	403	GLY	3.8
1	K	46	GLN	3.7
1	J	51	ARG	3.7
1	P	154	SER	3.7
1	I	16	ARG	3.7
1	C	282	GLY	3.7
1	I	52	GLY	3.7
1	I	51	ARG	3.7
1	L	395	ARG	3.7
1	G	295	VAL	3.6
1	M	55	VAL	3.6
1	C	287	MET	3.6
1	K	293	ALA	3.6
1	B	39	PRO	3.6
1	P	46	GLN	3.6
1	L	153	CYS	3.6
1	N	41	ASP	3.6
1	N	54	THR	3.6
1	N	255	GLU	3.6
1	I	14	LEU	3.6
1	P	285	PHE	3.6
1	G	46	GLN	3.6
1	G	155	CYS	3.6
1	H	286	GLY	3.6
1	I	196	ALA	3.5
1	J	44	ASN	3.5
1	N	405	LEU	3.5
1	I	49	ASP	3.5
1	J	369	VAL	3.5
1	J	22	HIS	3.5
1	O	392	GLU	3.5
1	L	283	ALA	3.5
1	L	409	GLN	3.5
1	L	347	LEU	3.5
1	I	287	MET	3.5
1	I	17	GLY	3.5
1	N	39	PRO	3.5
1	G	290	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	N	47	ALA	3.5
1	N	307	GLU	3.5
1	A	153	CYS	3.4
1	I	294	LYS	3.4
1	K	45	ALA	3.4
1	K	254	ASP	3.4
1	L	49	ASP	3.4
1	K	297	SER	3.4
1	L	43	PRO	3.4
1	M	6	LEU	3.4
1	K	283	ALA	3.4
1	I	43	PRO	3.4
1	N	297	SER	3.4
1	P	282	GLY	3.4
1	F	41	ASP	3.3
1	P	295	VAL	3.3
1	M	338	ALA	3.3
1	L	3	ILE	3.3
1	J	398	TYR	3.3
1	N	26	VAL	3.3
1	N	298	VAL	3.3
1	M	42	LEU	3.3
1	M	278	LEU	3.3
1	C	28	ASP	3.3
1	I	4	THR	3.3
1	M	37	ASP	3.3
1	P	41	ASP	3.3
1	I	384	GLU	3.3
1	M	156	CYS	3.3
1	I	42	LEU	3.3
1	N	22	HIS	3.3
1	I	47	ALA	3.3
1	L	46	GLN	3.3
1	K	195	VAL	3.3
1	N	290	GLU	3.3
1	K	28	ASP	3.3
1	K	199	THR	3.2
1	M	18	VAL	3.2
1	G	286	GLY	3.2
1	P	286	GLY	3.2
1	I	53	LYS	3.2
1	J	50	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	277	ALA	3.2
1	D	391	ASP	3.2
1	I	282	GLY	3.2
1	J	254	ASP	3.2
1	K	279	ALA	3.2
1	I	290	GLU	3.2
1	N	12	LEU	3.2
1	L	370	GLY	3.2
1	N	388	VAL	3.2
1	I	394	ALA	3.2
1	F	42	LEU	3.2
1	K	33	VAL	3.2
1	L	392	GLU	3.2
1	N	292	VAL	3.2
1	G	297	SER	3.2
1	J	7	GLN	3.1
1	G	292	VAL	3.1
1	J	55	VAL	3.1
1	K	19	LEU	3.1
1	K	260	LEU	3.1
1	P	38	ARG	3.1
1	K	289	PRO	3.1
1	I	3	ILE	3.1
1	K	278	LEU	3.1
1	K	383	LEU	3.1
1	K	38	ARG	3.1
1	L	282	GLY	3.1
1	I	153	CYS	3.1
1	L	382	PRO	3.1
1	F	38	ARG	3.1
1	M	36	THR	3.1
1	J	381	ASN	3.1
1	N	25	VAL	3.1
1	C	51	ARG	3.0
1	M	195	VAL	3.0
1	M	408	ARG	3.0
1	O	290	GLU	3.0
1	N	203	ALA	3.0
1	L	398	TYR	3.0
1	N	400	LEU	3.0
1	P	293	ALA	3.0
1	L	304	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	155	CYS	3.0
1	K	314	VAL	3.0
1	L	48	ILE	3.0
1	L	51	ARG	3.0
1	P	408	ARG	3.0
1	M	20	LEU	3.0
1	P	292	VAL	3.0
1	C	3	ILE	2.9
1	A	38	ARG	2.9
1	P	279	ALA	2.9
1	J	391	ASP	2.9
1	O	285	PHE	2.9
1	M	383	LEU	2.9
1	I	292	VAL	2.9
1	L	40	VAL	2.9
1	H	44	ASN	2.9
1	K	154	SER	2.9
1	M	46	GLN	2.9
1	M	11	VAL	2.9
1	L	41	ASP	2.9
1	K	47	ALA	2.9
1	J	28	ASP	2.9
1	L	39	PRO	2.9
1	M	41	ASP	2.9
1	I	45	ALA	2.9
1	P	152	PRO	2.9
1	I	24	HIS	2.9
1	J	26	VAL	2.9
1	L	408	ARG	2.9
1	O	42	LEU	2.8
1	C	295	VAL	2.8
1	J	288	PRO	2.8
1	M	394	ALA	2.8
1	M	281	HIS	2.8
1	I	398	TYR	2.8
1	I	297	SER	2.8
1	J	361	GLN	2.8
1	K	26	VAL	2.8
1	N	378	LEU	2.8
1	I	283	ALA	2.8
1	M	376	VAL	2.8
1	I	300	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	370	GLY	2.8
1	L	152	PRO	2.8
1	O	39	PRO	2.8
1	N	398	TYR	2.8
1	E	39	PRO	2.8
1	O	40	VAL	2.8
1	G	41	ASP	2.8
1	H	51	ARG	2.8
1	N	24	HIS	2.7
1	K	37	ASP	2.7
1	J	53	LYS	2.7
1	N	344	LEU	2.7
1	K	16	ARG	2.7
1	L	343	ASN	2.7
1	J	284	GLU	2.7
1	D	284	GLU	2.7
1	M	388	VAL	2.7
1	J	362	GLY	2.7
1	M	38	ARG	2.7
1	I	46	GLN	2.7
1	J	3	ILE	2.7
1	A	295	VAL	2.7
1	J	367	ILE	2.7
1	L	289	PRO	2.7
1	M	16	ARG	2.7
1	L	14	LEU	2.7
1	N	10	ASN	2.7
1	K	284	GLU	2.7
1	M	279	ALA	2.7
1	P	281	HIS	2.7
1	L	278	LEU	2.7
1	L	285	PHE	2.7
1	L	27	ILE	2.7
1	P	392	GLU	2.7
1	G	293	ALA	2.7
1	O	283	ALA	2.7
1	N	48	ILE	2.7
1	F	154	SER	2.7
1	I	198	PRO	2.6
1	I	36	THR	2.6
1	G	289	PRO	2.6
1	M	283	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	51	ARG	2.6
1	L	266	ALA	2.6
1	E	40	VAL	2.6
1	I	21	GLU	2.6
1	K	280	LYS	2.6
1	K	292	VAL	2.6
1	G	154	SER	2.6
1	E	38	ARG	2.6
1	M	399	VAL	2.6
1	A	393	GLY	2.6
1	M	284	GLU	2.6
1	I	199	THR	2.6
1	J	49	ASP	2.6
1	G	284	GLU	2.6
1	J	29	GLY	2.6
1	J	47	ALA	2.6
1	M	377	VAL	2.6
1	J	16	ARG	2.6
1	J	281	HIS	2.6
1	K	369	VAL	2.6
1	I	393	GLY	2.6
1	B	2	THR	2.5
1	L	391	ASP	2.5
1	L	45	ALA	2.5
1	K	29	GLY	2.5
1	L	292	VAL	2.5
1	M	19	LEU	2.5
1	L	307	GLU	2.5
1	M	255	GLU	2.5
1	A	286	GLY	2.5
1	M	294	LYS	2.5
1	O	38	ARG	2.5
1	J	293	ALA	2.5
1	C	52	GLY	2.5
1	I	278	LEU	2.5
1	M	329	PHE	2.5
1	I	379	ASP	2.5
1	M	35	VAL	2.5
1	I	391	ASP	2.5
1	J	4	THR	2.5
1	L	372	ILE	2.5
1	L	295	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	62	CYS	2.5
1	L	6	LEU	2.5
1	L	405	LEU	2.5
1	C	291	SER	2.5
1	L	31	ARG	2.5
1	L	404	THR	2.4
1	J	21	GLU	2.4
1	P	319	GLY	2.4
1	N	50	VAL	2.4
1	J	70	ASN	2.4
1	M	62	CYS	2.4
1	J	20	LEU	2.4
1	L	21	GLU	2.4
1	K	44	ASN	2.4
1	N	409	GLN	2.4
1	E	319	GLY	2.4
1	K	51	ARG	2.4
1	I	405	LEU	2.4
1	I	291	SER	2.4
1	K	52	GLY	2.4
1	H	290	GLU	2.4
1	B	42	LEU	2.4
1	B	46	GLN	2.4
1	M	286	GLY	2.4
1	I	397	GLU	2.4
1	J	30	GLU	2.4
1	J	397	GLU	2.4
1	L	30	GLU	2.4
1	L	57	PRO	2.4
1	J	400	LEU	2.4
1	K	12	LEU	2.4
1	M	301	LYS	2.4
1	G	16	ARG	2.4
1	J	255	GLU	2.4
1	N	55	VAL	2.4
1	J	32	ILE	2.3
1	K	384	GLU	2.3
1	P	16	ARG	2.3
1	N	406	VAL	2.3
1	K	53	LYS	2.3
1	M	369	VAL	2.3
1	K	255	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	155	CYS	2.3
1	J	282	GLY	2.3
1	M	313	GLY	2.3
1	I	19	LEU	2.3
1	L	10	ASN	2.3
1	L	42	LEU	2.3
1	O	292	VAL	2.3
1	F	409	GLN	2.3
1	N	377	VAL	2.3
1	L	280	LYS	2.3
1	J	23	HIS	2.3
1	P	43	PRO	2.3
1	E	392	GLU	2.3
1	O	398	TYR	2.3
1	B	38	ARG	2.3
1	E	3	ILE	2.3
1	M	385	ASP	2.3
1	I	44	ASN	2.2
1	J	36	THR	2.2
1	K	27	ILE	2.2
1	P	317	GLY	2.2
1	P	260	LEU	2.2
1	O	2	THR	2.2
1	L	50	VAL	2.2
1	J	34	GLU	2.2
1	A	289	PRO	2.2
1	C	281	HIS	2.2
1	K	264	HIS	2.2
1	L	22	HIS	2.2
1	N	53	LYS	2.2
1	P	198	PRO	2.2
1	J	257	ALA	2.2
1	P	153	CYS	2.2
1	K	22	HIS	2.2
1	P	288	PRO	2.2
1	N	279	ALA	2.2
1	L	379	ASP	2.2
1	L	385	ASP	2.2
1	I	9	GLY	2.2
1	M	29	GLY	2.2
1	K	3	ILE	2.2
1	K	5	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	32	ILE	2.2
1	F	16	ARG	2.2
1	M	311	ASN	2.2
1	A	42	LEU	2.2
1	M	24	HIS	2.2
1	E	320	SER	2.2
1	M	154	SER	2.2
1	M	340	VAL	2.2
1	F	289	PRO	2.2
1	K	41	ASP	2.2
1	L	47	ALA	2.2
1	M	4	THR	2.2
1	L	55	VAL	2.2
1	N	280	LYS	2.2
1	B	289	PRO	2.1
1	N	19	LEU	2.1
1	D	28	ASP	2.1
1	O	36	THR	2.1
1	O	51	ARG	2.1
1	A	285	PHE	2.1
1	F	15	GLU	2.1
1	L	24	HIS	2.1
1	O	43	PRO	2.1
1	O	52	GLY	2.1
1	M	287	MET	2.1
1	O	384	GLU	2.1
1	K	240	VAL	2.1
1	J	37	ASP	2.1
1	J	395	ARG	2.1
1	O	361	GLN	2.1
1	G	62	CYS	2.1
1	L	344	LEU	2.1
1	K	296	ALA	2.1
1	J	31	ARG	2.1
1	F	292	VAL	2.1
1	H	292	VAL	2.1
1	G	288	PRO	2.1
1	N	288	PRO	2.1
1	E	2	THR	2.1
1	B	290	GLU	2.1
1	K	11	VAL	2.1
1	D	409	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	392	GLU	2.1
1	E	48	ILE	2.1
1	J	33	VAL	2.1
1	O	298	VAL	2.1
1	P	63	HIS	2.1
1	C	155	CYS	2.1
1	D	155	CYS	2.1
1	G	153	CYS	2.1
1	K	234	ARG	2.1
1	H	287	MET	2.1
1	N	202	ILE	2.0
1	L	311	ASN	2.0
1	P	320	SER	2.0
1	N	285	PHE	2.0
1	N	367	ILE	2.0
1	C	392	GLU	2.0
1	J	311	ASN	2.0
1	B	286	GLY	2.0
1	N	282	GLY	2.0
1	N	294	LYS	2.0
1	L	5	VAL	2.0
1	M	52	GLY	2.0
1	P	106	ALA	2.0
1	P	409	GLN	2.0
1	C	285	PHE	2.0
1	M	15	GLU	2.0
1	N	399	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	C	425	1/1	0.97	0.29	7.37	42,42,42,42	1
2	ZN	J	426	1/1	0.95	0.31	5.26	68,68,68,68	1
2	ZN	L	426	1/1	0.94	0.31	4.22	63,63,63,63	1
2	ZN	O	425	1/1	0.96	0.31	4.18	50,50,50,50	1
2	ZN	L	425	1/1	0.93	0.28	4.02	55,55,55,55	1
2	ZN	E	426	1/1	0.94	0.40	4.00	45,45,45,45	1
2	ZN	D	426	1/1	0.93	0.32	3.48	33,33,33,33	1
2	ZN	C	426	1/1	0.96	0.27	3.14	38,38,38,38	1
2	ZN	N	426	1/1	0.89	0.31	3.08	55,55,55,55	1
2	ZN	F	426	1/1	0.84	0.32	3.02	51,51,51,51	1
2	ZN	M	426	1/1	0.93	0.36	3.02	63,63,63,63	1
2	ZN	O	426	1/1	0.85	0.29	2.87	58,58,58,58	1
2	ZN	P	426	1/1	0.95	0.38	2.69	59,59,59,59	1
2	ZN	J	425	1/1	0.93	0.24	2.67	60,60,60,60	1
2	ZN	H	425	1/1	0.98	0.28	2.49	40,40,40,40	1
2	ZN	N	425	1/1	0.88	0.29	2.39	41,41,41,41	1
2	ZN	A	426	1/1	0.96	0.23	1.98	52,52,52,52	1
2	ZN	H	426	1/1	0.95	0.29	1.97	39,39,39,39	1
2	ZN	A	425	1/1	0.98	0.25	1.79	51,51,51,51	1
2	ZN	G	425	1/1	0.97	0.27	1.79	40,40,40,40	1
2	ZN	I	425	1/1	0.97	0.20	1.69	42,42,42,42	1
2	ZN	F	425	1/1	0.95	0.27	1.60	52,52,52,52	1
2	ZN	B	425	1/1	0.95	0.26	1.49	44,44,44,44	1
2	ZN	B	426	1/1	0.97	0.25	1.48	44,44,44,44	1
2	ZN	E	425	1/1	0.97	0.28	1.33	43,43,43,43	1
2	ZN	I	426	1/1	0.84	0.19	1.31	58,58,58,58	1
2	ZN	G	426	1/1	0.98	0.24	1.02	37,37,37,37	1
2	ZN	P	425	1/1	0.88	0.30	0.99	47,47,47,47	1
2	ZN	K	425	1/1	0.92	0.23	0.84	55,55,55,55	1
2	ZN	D	425	1/1	0.95	0.21	0.29	34,34,34,34	1
2	ZN	K	426	1/1	0.95	0.12	-1.57	68,68,68,68	1
2	ZN	M	425	1/1	0.88	0.21	-1.75	50,50,50,50	1

6.5 Other polymers ⓘ

There are no such residues in this entry.