



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:07 AM UTC

PDB ID : 4OYE / pdb_00004oye
Title : Crystal structure of GltPh R397A in apo
Authors : Boudker, O.; Oh, S.
Deposited on : 2014-02-11
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

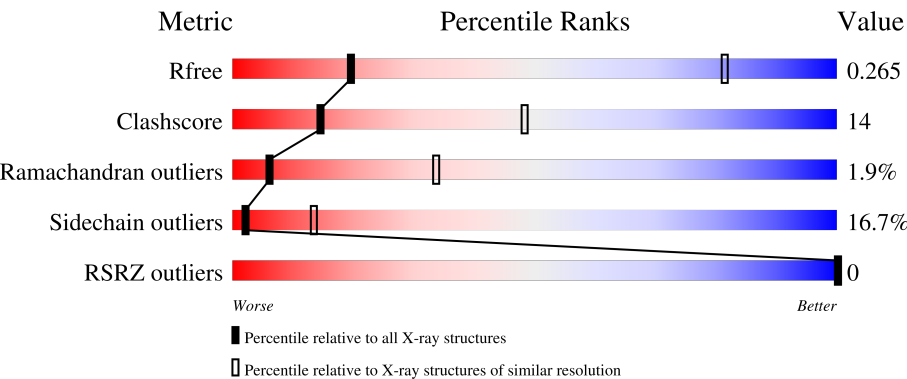
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	409	63%28%6% .
1	B	409	66%25%7% .
1	C	409	64%29%5% .
1	D	409	66%27%6% .
1	E	409	67%25%7% .

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Mol	Chain	Length	Quality of chain
1	F	409	 67%25%6% .
1	G	409	 67%25%6% .
1	H	409	 66%26%7% .
1	I	409	 64%27%7% .
1	J	409	 66%26%6% .
1	K	409	 66%26%7% .
1	L	409	 66%25%7% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 35277 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 425aa long hypothetical proton glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			2925	1930	465	513	17			
1	B	404	Total	C	N	O	S	0	0	0
			2939	1938	468	516	17			
1	C	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	D	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	E	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	F	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	G	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	H	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	I	403	Total	C	N	O	S	0	0	0
			2934	1935	467	515	17			
1	J	404	Total	C	N	O	S	0	0	0
			2943	1940	469	517	17			
1	K	404	Total	C	N	O	S	0	0	0
			2939	1937	468	517	17			
1	L	404	Total	C	N	O	S	0	0	0
			2939	1938	469	515	17			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010

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Chain	Residue	Modelled	Actual	Comment	Reference
A	368	HIS	GLU	engineered mutation	UNP O59010
A	397	ALA	ARG	engineered mutation	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	368	HIS	GLU	engineered mutation	UNP O59010
B	397	ALA	ARG	engineered mutation	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	397	ALA	ARG	engineered mutation	UNP O59010
D	37	HIS	ASP	engineered mutation	UNP O59010
D	40	HIS	LYS	engineered mutation	UNP O59010
D	132	HIS	LYS	engineered mutation	UNP O59010
D	223	HIS	LYS	engineered mutation	UNP O59010
D	264	HIS	LYS	engineered mutation	UNP O59010
D	368	HIS	GLU	engineered mutation	UNP O59010
D	397	ALA	ARG	engineered mutation	UNP O59010
E	37	HIS	ASP	engineered mutation	UNP O59010
E	40	HIS	LYS	engineered mutation	UNP O59010
E	132	HIS	LYS	engineered mutation	UNP O59010
E	223	HIS	LYS	engineered mutation	UNP O59010
E	264	HIS	LYS	engineered mutation	UNP O59010
E	368	HIS	GLU	engineered mutation	UNP O59010
E	397	ALA	ARG	engineered mutation	UNP O59010
F	37	HIS	ASP	engineered mutation	UNP O59010
F	40	HIS	LYS	engineered mutation	UNP O59010
F	132	HIS	LYS	engineered mutation	UNP O59010
F	223	HIS	LYS	engineered mutation	UNP O59010
F	264	HIS	LYS	engineered mutation	UNP O59010
F	368	HIS	GLU	engineered mutation	UNP O59010
F	397	ALA	ARG	engineered mutation	UNP O59010
G	37	HIS	ASP	engineered mutation	UNP O59010
G	40	HIS	LYS	engineered mutation	UNP O59010
G	132	HIS	LYS	engineered mutation	UNP O59010
G	223	HIS	LYS	engineered mutation	UNP O59010
G	264	HIS	LYS	engineered mutation	UNP O59010

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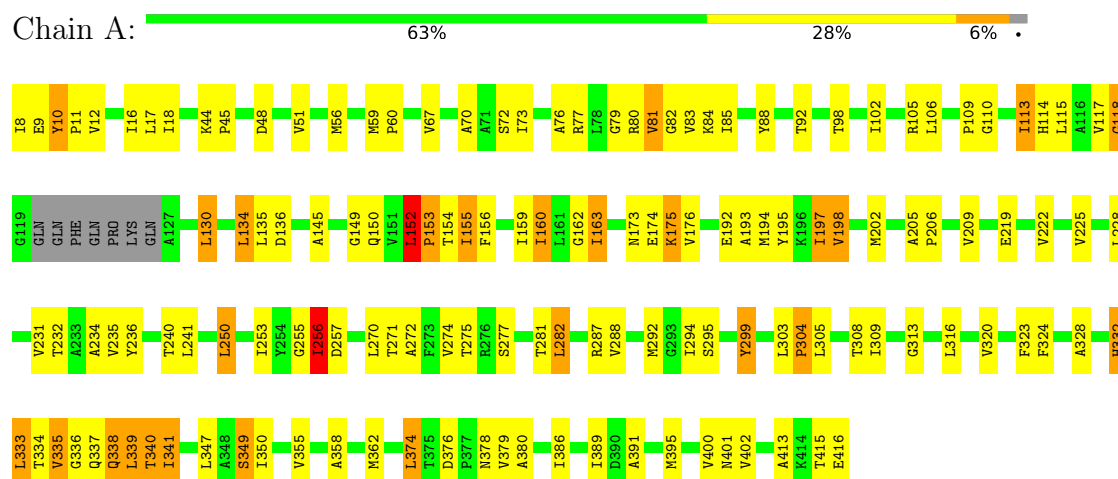
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Chain	Residue	Modelled	Actual	Comment	Reference
G	368	HIS	GLU	engineered mutation	UNP O59010
G	397	ALA	ARG	engineered mutation	UNP O59010
H	37	HIS	ASP	engineered mutation	UNP O59010
H	40	HIS	LYS	engineered mutation	UNP O59010
H	132	HIS	LYS	engineered mutation	UNP O59010
H	223	HIS	LYS	engineered mutation	UNP O59010
H	264	HIS	LYS	engineered mutation	UNP O59010
H	368	HIS	GLU	engineered mutation	UNP O59010
H	397	ALA	ARG	engineered mutation	UNP O59010
I	37	HIS	ASP	engineered mutation	UNP O59010
I	40	HIS	LYS	engineered mutation	UNP O59010
I	132	HIS	LYS	engineered mutation	UNP O59010
I	223	HIS	LYS	engineered mutation	UNP O59010
I	264	HIS	LYS	engineered mutation	UNP O59010
I	368	HIS	GLU	engineered mutation	UNP O59010
I	397	ALA	ARG	engineered mutation	UNP O59010
J	37	HIS	ASP	engineered mutation	UNP O59010
J	40	HIS	LYS	engineered mutation	UNP O59010
J	132	HIS	LYS	engineered mutation	UNP O59010
J	223	HIS	LYS	engineered mutation	UNP O59010
J	264	HIS	LYS	engineered mutation	UNP O59010
J	368	HIS	GLU	engineered mutation	UNP O59010
J	397	ALA	ARG	engineered mutation	UNP O59010
K	37	HIS	ASP	engineered mutation	UNP O59010
K	40	HIS	LYS	engineered mutation	UNP O59010
K	132	HIS	LYS	engineered mutation	UNP O59010
K	223	HIS	LYS	engineered mutation	UNP O59010
K	264	HIS	LYS	engineered mutation	UNP O59010
K	368	HIS	GLU	engineered mutation	UNP O59010
K	397	ALA	ARG	engineered mutation	UNP O59010
L	37	HIS	ASP	engineered mutation	UNP O59010
L	40	HIS	LYS	engineered mutation	UNP O59010
L	132	HIS	LYS	engineered mutation	UNP O59010
L	223	HIS	LYS	engineered mutation	UNP O59010
L	264	HIS	LYS	engineered mutation	UNP O59010
L	368	HIS	GLU	engineered mutation	UNP O59010
L	397	ALA	ARG	engineered mutation	UNP O59010

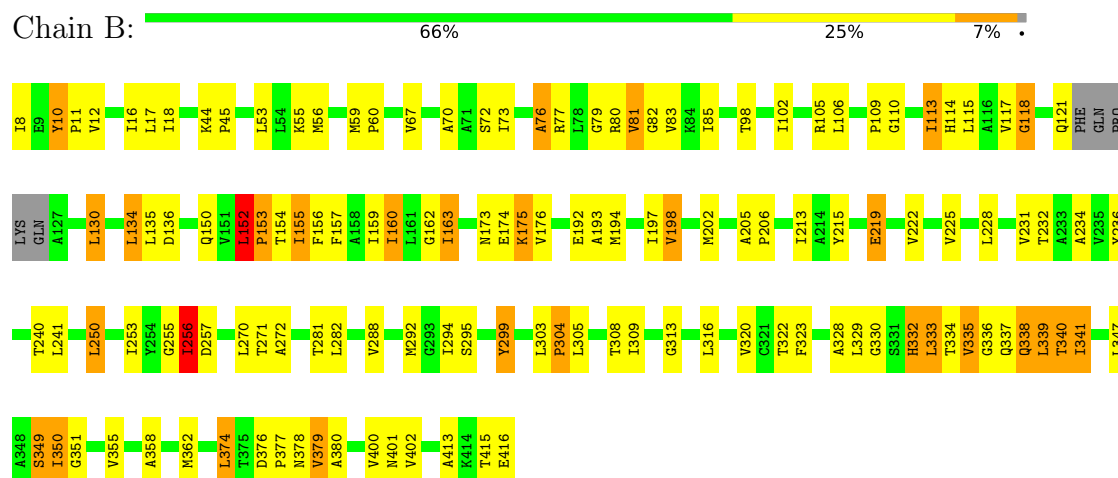
3 Residue-property plots

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: 425aa long hypothetical proton glutamate symport protein

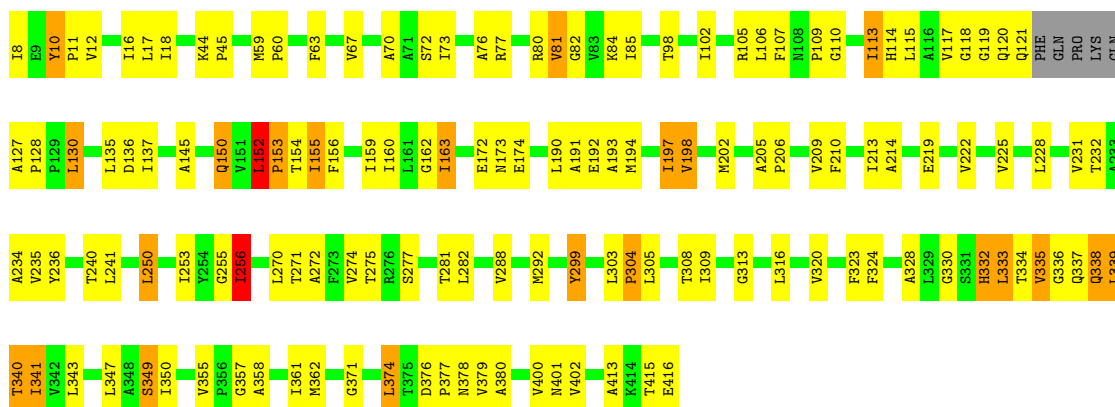


- Molecule 1: 425aa long hypothetical proton glutamate symport protein



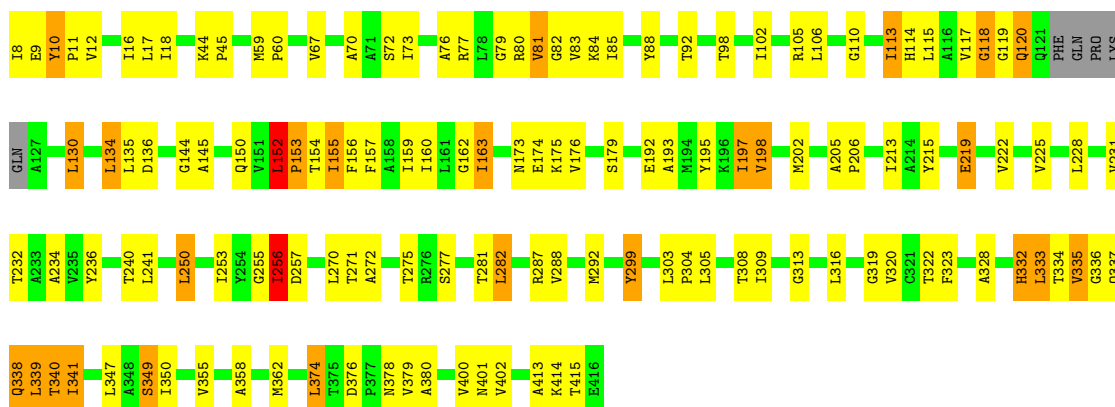
- Molecule 1: 425aa long hypothetical proton glutamate symport protein





- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain D: 66% 27% 6% •



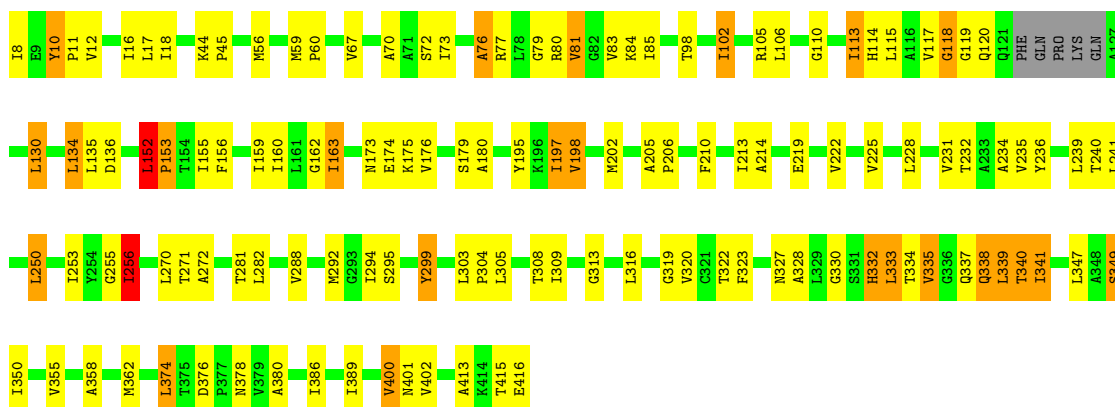
- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain E: 67% 25% 7% •

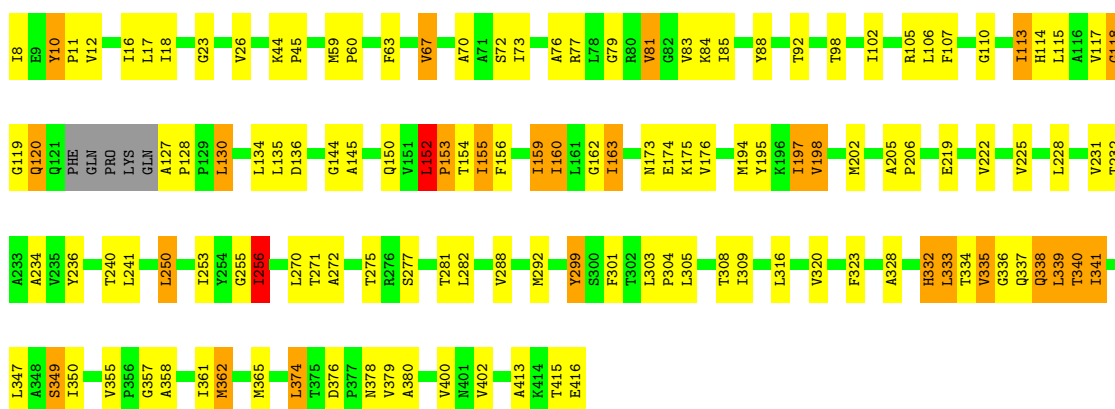


- Molecule 1: 425aa long hypothetical proton glutamate symport protein

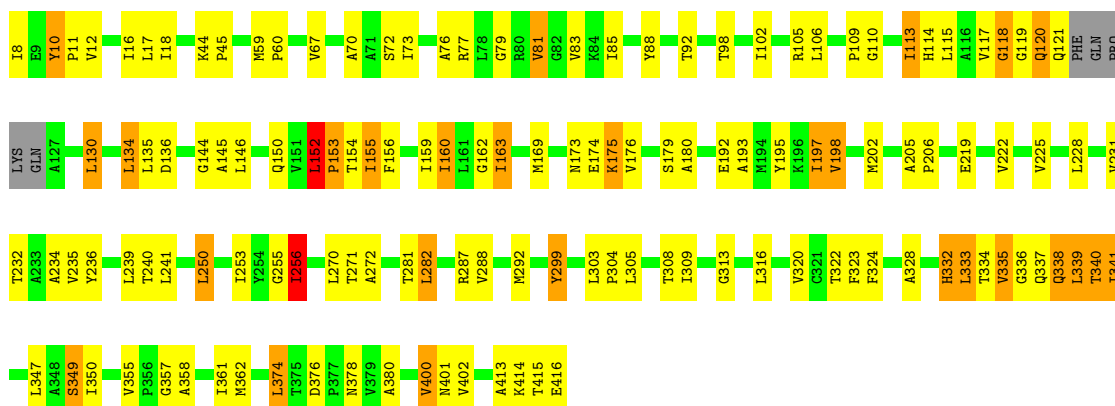
Chain F: 67% 25% 6% •



- Molecule 1: 425aa long hypothetical proton glutamate symport protein

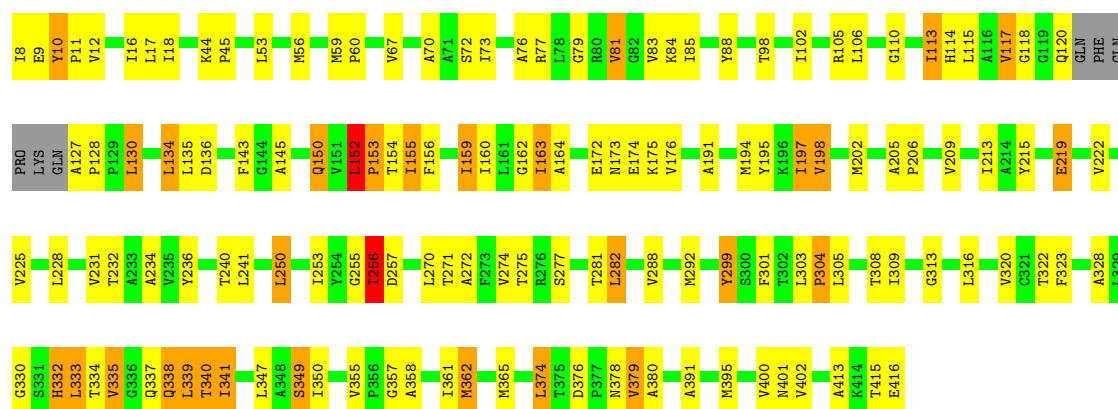


- Molecule 1: 425aa long hypothetical proton glutamate symport protein



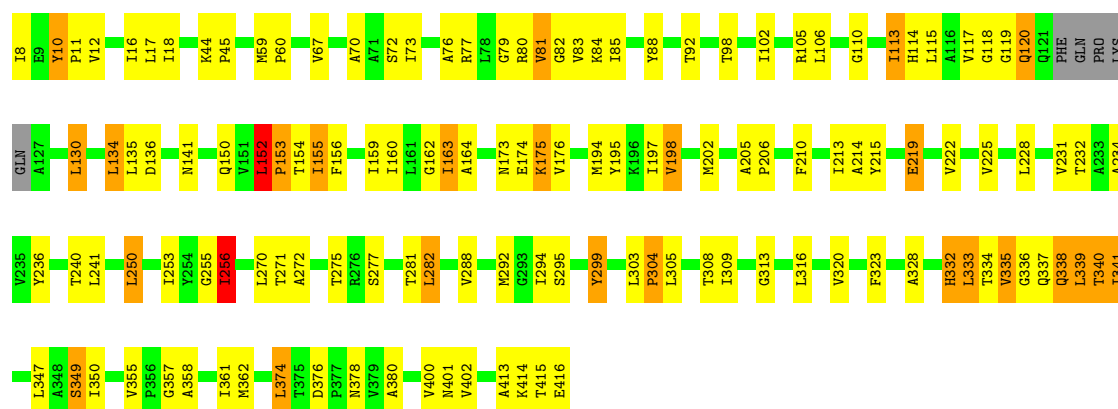
- Molecule 1: 425aa long hypothetical proton glutamate symport protein





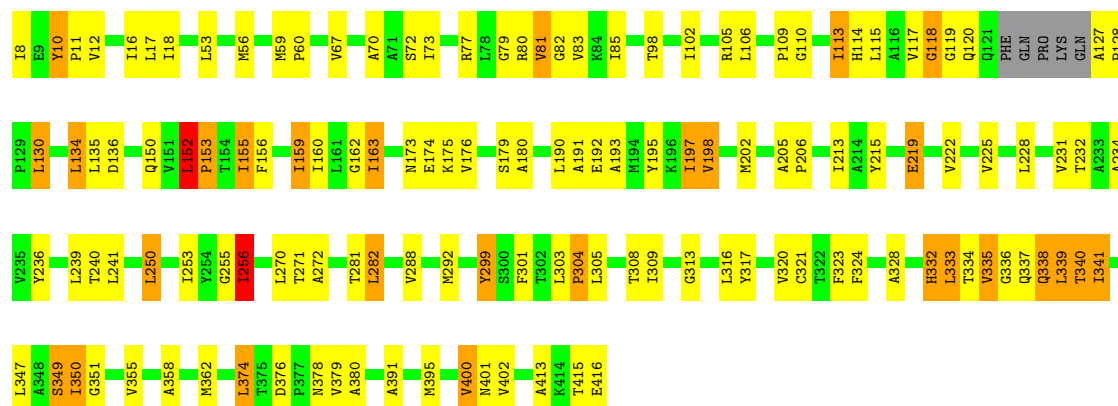
- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain J: 66% 26% 6% •



- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain K: 66% 26% 7% •



- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain L: 66% 25% 7% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.36Å 424.42Å 113.98Å 90.00° 119.38° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 20.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	70.3 (20.00-4.00) 70.4 (20.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 4.07Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.249 , 0.266 0.250 , 0.265	Depositor DCC
R_{free} test set	2728 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	1.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.068 for -h-l,k,h 0.068 for l,k,-h-l 0.208 for h,-k,-h-l 0.078 for -h-l,-k,l 0.076 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35277	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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

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	0.74	0/2980	0.98	4/4074 (0.1%)
1	B	0.85	1/2994 (0.0%)	1.01	7/4093 (0.2%)
1	C	0.82	0/2998	1.00	0/4098
1	D	0.74	0/2998	0.98	3/4098 (0.1%)
1	E	0.78	0/2998	0.97	1/4098 (0.0%)
1	F	0.84	0/2998	1.00	2/4098 (0.0%)
1	G	0.77	0/2998	0.98	1/4098 (0.0%)
1	H	0.74	0/2998	0.98	2/4098 (0.0%)
1	I	0.79	0/2989	1.01	5/4086 (0.1%)
1	J	0.69	0/2998	0.99	2/4098 (0.0%)
1	K	0.77	0/2994	0.98	1/4094 (0.0%)
1	L	0.83	0/2994	0.99	5/4093 (0.1%)
All	All	0.78	1/35937 (0.0%)	0.99	33/49126 (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	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	PRO	CA-C	6.62	1.60	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	VAL	N-CA-C	-7.73	103.26	110.53
1	L	67	VAL	N-CA-C	-7.13	103.83	110.53
1	J	67	VAL	N-CA-C	-7.07	103.89	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	VAL	N-CA-C	-6.79	104.14	110.53
1	D	67	VAL	N-CA-C	-6.61	104.32	110.53
1	H	67	VAL	N-CA-C	-6.28	104.63	110.53
1	G	67	VAL	N-CA-C	-5.89	104.99	110.53
1	H	175	LYS	N-CA-C	-5.78	104.58	111.69
1	K	67	VAL	N-CA-C	-5.75	105.12	110.53
1	I	379	VAL	N-CA-C	-5.65	104.82	110.30
1	B	175	LYS	N-CA-C	-5.62	104.78	111.69
1	B	379	VAL	N-CA-C	-5.55	104.92	110.30
1	I	67	VAL	N-CA-C	-5.51	105.35	110.53
1	I	257	ASP	CA-C-N	5.37	124.83	119.24
1	I	257	ASP	C-N-CA	5.37	124.83	119.24
1	F	67	VAL	N-CA-C	-5.37	105.48	110.53
1	L	128	PRO	N-CA-C	5.32	117.19	110.70
1	B	329	LEU	N-CA-C	-5.31	107.10	113.21
1	L	329	LEU	N-CA-C	-5.25	107.18	113.21
1	I	117	VAL	N-CA-C	5.18	115.95	107.24
1	A	175	LYS	N-CA-C	-5.16	105.34	111.69
1	L	257	ASP	CA-C-N	5.16	124.60	119.24
1	L	257	ASP	C-N-CA	5.16	124.60	119.24
1	B	257	ASP	CA-C-N	5.15	124.60	119.24
1	B	257	ASP	C-N-CA	5.15	124.60	119.24
1	E	107	PHE	N-CA-C	-5.13	102.88	110.48
1	F	76	ALA	N-CA-C	-5.12	102.42	110.36
1	D	257	ASP	CA-C-N	5.12	124.56	119.24
1	D	257	ASP	C-N-CA	5.12	124.56	119.24
1	B	76	ALA	N-CA-C	-5.10	102.45	110.36
1	J	175	LYS	N-CA-C	-5.06	105.47	111.69
1	A	257	ASP	CA-C-N	5.06	124.50	119.24
1	A	257	ASP	C-N-CA	5.06	124.50	119.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	174	GLU	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	2925	0	3069	88	0
1	B	2939	0	3079	84	0
1	C	2943	0	3085	100	0
1	D	2943	0	3085	84	0
1	E	2943	0	3085	79	0
1	F	2943	0	3085	82	0
1	G	2943	0	3085	86	0
1	H	2943	0	3085	84	0
1	I	2934	0	3077	94	0
1	J	2943	0	3085	80	0
1	K	2939	0	3074	85	0
1	L	2939	0	3081	87	0
All	All	35277	0	36975	1013	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1013) 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:C:73:ILE:CD1	1:I:172:GLU:CB	2.19	1.19
1:C:73:ILE:HD13	1:I:172:GLU:CB	1.79	1.12
1:C:73:ILE:HD11	1:I:172:GLU:CB	2.03	0.89
1:B:338:GLN:O	1:B:341:ILE:HD13	1.81	0.80
1:F:338:GLN:O	1:F:341:ILE:HD13	1.85	0.75
1:K:338:GLN:O	1:K:341:ILE:HD13	1.85	0.75
1:A:338:GLN:O	1:A:341:ILE:HD13	1.85	0.75
1:G:338:GLN:O	1:G:341:ILE:HD13	1.86	0.74
1:H:338:GLN:O	1:H:341:ILE:HD13	1.87	0.74
1:L:338:GLN:O	1:L:341:ILE:HD13	1.88	0.74
1:D:338:GLN:O	1:D:341:ILE:HD13	1.88	0.74
1:J:338:GLN:O	1:J:341:ILE:HD13	1.86	0.74
1:E:338:GLN:O	1:E:341:ILE:HD13	1.88	0.74
1:I:338:GLN:O	1:I:341:ILE:HD13	1.87	0.74
1:C:338:GLN:O	1:C:341:ILE:HD13	1.89	0.73
1:E:117:VAL:HG11	1:E:378:ASN:HB2	1.72	0.70
1:G:117:VAL:HG11	1:G:378:ASN:HB2	1.72	0.70
1:J:117:VAL:HG11	1:J:378:ASN:HB2	1.73	0.70
1:K:117:VAL:HG11	1:K:378:ASN:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:117:VAL:HG11	1:I:378:ASN:HB2	1.74	0.69
1:F:117:VAL:HG11	1:F:378:ASN:HB2	1.74	0.69
1:L:117:VAL:HG11	1:L:378:ASN:HB2	1.72	0.68
1:C:117:VAL:HG11	1:C:378:ASN:HB2	1.75	0.68
1:D:117:VAL:HG11	1:D:378:ASN:HB2	1.75	0.68
1:B:117:VAL:HG11	1:B:378:ASN:HB2	1.74	0.68
1:C:70:ALA:HB3	1:C:162:GLY:HA3	1.75	0.68
1:D:70:ALA:HB3	1:D:162:GLY:HA3	1.76	0.67
1:A:117:VAL:HG11	1:A:378:ASN:HB2	1.77	0.67
1:H:117:VAL:HG11	1:H:378:ASN:HB2	1.75	0.67
1:I:349:SER:O	1:I:349:SER:OG	2.12	0.67
1:A:10:TYR:HB3	1:A:11:PRO:HD2	1.78	0.66
1:C:10:TYR:HB3	1:C:11:PRO:HD2	1.78	0.66
1:L:10:TYR:HB3	1:L:11:PRO:HD2	1.77	0.65
1:G:10:TYR:HB3	1:G:11:PRO:HD2	1.78	0.65
1:F:10:TYR:HB3	1:F:11:PRO:HD2	1.79	0.65
1:J:70:ALA:HB3	1:J:162:GLY:HA3	1.79	0.65
1:B:10:TYR:HB3	1:B:11:PRO:HD2	1.77	0.65
1:G:77:ARG:HD3	1:G:416:GLU:HG2	1.79	0.65
1:J:10:TYR:HB3	1:J:11:PRO:HD2	1.78	0.65
1:E:10:TYR:HB3	1:E:11:PRO:HD2	1.79	0.64
1:H:10:TYR:HB3	1:H:11:PRO:HD2	1.79	0.64
1:B:288:VAL:O	1:B:292:MET:HB2	1.98	0.64
1:K:10:TYR:HB3	1:K:11:PRO:HD2	1.79	0.64
1:I:70:ALA:HB3	1:I:162:GLY:HA3	1.79	0.64
1:L:70:ALA:HB3	1:L:162:GLY:HA3	1.80	0.64
1:B:70:ALA:HB3	1:B:162:GLY:HA3	1.81	0.63
1:D:288:VAL:O	1:D:292:MET:HB2	1.99	0.63
1:E:70:ALA:HB3	1:E:162:GLY:HA3	1.79	0.63
1:H:288:VAL:O	1:H:292:MET:HB2	1.99	0.63
1:C:73:ILE:CG1	1:I:172:GLU:CB	2.77	0.63
1:F:113:ILE:O	1:F:328:ALA:HA	1.99	0.63
1:A:288:VAL:O	1:A:292:MET:HB2	1.98	0.63
1:F:349:SER:O	1:F:349:SER:OG	2.13	0.63
1:B:77:ARG:HD3	1:B:416:GLU:HG2	1.81	0.63
1:I:77:ARG:HD3	1:I:416:GLU:HG2	1.81	0.63
1:F:70:ALA:HB3	1:F:162:GLY:HA3	1.80	0.63
1:H:349:SER:O	1:H:349:SER:OG	2.16	0.63
1:K:355:VAL:HG13	1:K:358:ALA:HB2	1.80	0.62
1:D:105:ARG:NH2	1:D:338:GLN:HB2	2.14	0.62
1:I:288:VAL:O	1:I:292:MET:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:ALA:HB3	1:G:162:GLY:HA3	1.80	0.62
1:I:10:TYR:HB3	1:I:11:PRO:HD2	1.81	0.62
1:K:105:ARG:NH2	1:K:338:GLN:HB2	2.15	0.62
1:C:349:SER:O	1:C:349:SER:OG	2.14	0.62
1:E:288:VAL:O	1:E:292:MET:HB2	2.00	0.62
1:G:288:VAL:O	1:G:292:MET:HB2	1.99	0.62
1:J:288:VAL:O	1:J:292:MET:HB2	1.99	0.62
1:C:77:ARG:HD3	1:C:416:GLU:HG2	1.81	0.62
1:D:349:SER:O	1:D:349:SER:OG	2.17	0.62
1:A:105:ARG:NH2	1:A:338:GLN:HB2	2.14	0.62
1:H:355:VAL:HG13	1:H:358:ALA:HB2	1.81	0.62
1:E:105:ARG:NH2	1:E:338:GLN:HB2	2.15	0.61
1:F:105:ARG:NH2	1:F:338:GLN:HB2	2.14	0.61
1:K:77:ARG:HD3	1:K:416:GLU:HG2	1.82	0.61
1:G:105:ARG:NH2	1:G:338:GLN:HB2	2.15	0.61
1:C:288:VAL:O	1:C:292:MET:HB2	2.01	0.61
1:C:113:ILE:O	1:C:328:ALA:HA	2.01	0.61
1:L:334:THR:HB	1:L:337:GLN:HB3	1.82	0.61
1:A:70:ALA:HB3	1:A:162:GLY:HA3	1.83	0.61
1:C:172:GLU:CB	1:H:169:MET:HE1	2.30	0.61
1:K:155:ILE:HD11	1:K:304:PRO:HB2	1.82	0.61
1:D:10:TYR:HB3	1:D:11:PRO:HD2	1.81	0.61
1:H:105:ARG:NH2	1:H:338:GLN:HB2	2.15	0.61
1:I:105:ARG:NH2	1:I:338:GLN:HB2	2.15	0.61
1:F:113:ILE:HG22	1:F:115:LEU:HD13	1.83	0.61
1:A:113:ILE:CA	1:A:114:HIS:HB3	2.31	0.60
1:H:77:ARG:HD3	1:H:416:GLU:HG2	1.83	0.60
1:I:355:VAL:HG13	1:I:358:ALA:HB2	1.83	0.60
1:C:105:ARG:NH2	1:C:338:GLN:HB2	2.17	0.60
1:K:70:ALA:HB3	1:K:162:GLY:HA3	1.82	0.60
1:L:113:ILE:HG22	1:L:115:LEU:HD13	1.83	0.60
1:A:355:VAL:HG13	1:A:358:ALA:HB2	1.83	0.60
1:B:349:SER:O	1:B:349:SER:OG	2.13	0.60
1:H:70:ALA:HB3	1:H:162:GLY:HA3	1.81	0.60
1:L:105:ARG:NH2	1:L:338:GLN:HB2	2.14	0.60
1:E:355:VAL:HG13	1:E:358:ALA:HB2	1.82	0.60
1:E:119:GLY:N	1:E:120:GLN:HA	2.16	0.60
1:G:355:VAL:HG13	1:G:358:ALA:HB2	1.82	0.60
1:H:113:ILE:HG22	1:H:115:LEU:HD13	1.83	0.60
1:K:349:SER:OG	1:K:349:SER:O	2.20	0.60
1:A:334:THR:HB	1:A:337:GLN:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ARG:NH2	1:B:338:GLN:HB2	2.17	0.60
1:C:355:VAL:HG13	1:C:358:ALA:HB2	1.82	0.60
1:J:113:ILE:CA	1:J:114:HIS:HB3	2.32	0.59
1:J:271:THR:HG22	1:J:281:THR:HG22	1.84	0.59
1:L:113:ILE:CA	1:L:114:HIS:HB3	2.32	0.59
1:L:355:VAL:HG13	1:L:358:ALA:HB2	1.83	0.59
1:D:113:ILE:CA	1:D:114:HIS:HB3	2.31	0.59
1:F:334:THR:HB	1:F:337:GLN:HB3	1.84	0.59
1:I:113:ILE:HG22	1:I:115:LEU:HD13	1.83	0.59
1:J:105:ARG:NH2	1:J:338:GLN:HB2	2.16	0.59
1:E:271:THR:HG22	1:E:281:THR:HG22	1.83	0.59
1:E:349:SER:O	1:E:349:SER:OG	2.18	0.59
1:F:355:VAL:HG13	1:F:358:ALA:HB2	1.84	0.59
1:J:355:VAL:HG13	1:J:358:ALA:HB2	1.82	0.59
1:H:113:ILE:CA	1:H:114:HIS:HB3	2.32	0.59
1:F:113:ILE:CA	1:F:114:HIS:HB3	2.32	0.59
1:I:271:THR:HG22	1:I:281:THR:HG22	1.85	0.59
1:E:228:LEU:O	1:E:231:VAL:HG12	2.02	0.59
1:H:334:THR:HB	1:H:337:GLN:HB3	1.84	0.59
1:I:113:ILE:CA	1:I:114:HIS:HB3	2.33	0.59
1:K:288:VAL:O	1:K:292:MET:HB2	2.02	0.59
1:L:349:SER:O	1:L:349:SER:OG	2.19	0.59
1:E:155:ILE:HD11	1:E:304:PRO:HB2	1.83	0.59
1:L:271:THR:HG22	1:L:281:THR:HG22	1.83	0.59
1:B:228:LEU:O	1:B:231:VAL:HG12	2.02	0.59
1:F:155:ILE:HD11	1:F:304:PRO:HB2	1.85	0.59
1:K:228:LEU:O	1:K:231:VAL:HG12	2.03	0.59
1:B:355:VAL:HG13	1:B:358:ALA:HB2	1.83	0.58
1:H:155:ILE:HD11	1:H:304:PRO:HB2	1.85	0.58
1:B:271:THR:HG22	1:B:281:THR:HG22	1.84	0.58
1:D:355:VAL:HG13	1:D:358:ALA:HB2	1.84	0.58
1:L:155:ILE:HD11	1:L:304:PRO:HB2	1.86	0.58
1:A:113:ILE:HG22	1:A:115:LEU:HD13	1.85	0.58
1:B:334:THR:HB	1:B:337:GLN:HB3	1.84	0.58
1:C:334:THR:HB	1:C:337:GLN:HB3	1.86	0.58
1:B:113:ILE:CA	1:B:114:HIS:HB3	2.34	0.58
1:G:113:ILE:HG22	1:G:115:LEU:HD13	1.84	0.58
1:D:119:GLY:N	1:D:120:GLN:HA	2.19	0.58
1:E:113:ILE:CA	1:E:114:HIS:HB3	2.34	0.58
1:F:271:THR:HG22	1:F:281:THR:HG22	1.84	0.58
1:L:113:ILE:O	1:L:328:ALA:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ILE:HD11	1:B:304:PRO:HB2	1.86	0.58
1:F:113:ILE:HA	1:F:114:HIS:HB3	1.84	0.58
1:C:105:ARG:NE	1:C:335:VAL:HG13	2.19	0.58
1:I:155:ILE:HD11	1:I:304:PRO:HB2	1.85	0.58
1:K:113:ILE:CA	1:K:114:HIS:HB3	2.34	0.58
1:K:271:THR:HG22	1:K:281:THR:HG22	1.85	0.58
1:K:113:ILE:HG22	1:K:115:LEU:HD13	1.86	0.57
1:A:271:THR:HG22	1:A:281:THR:HG22	1.85	0.57
1:B:113:ILE:HG22	1:B:115:LEU:HD13	1.84	0.57
1:J:113:ILE:O	1:J:328:ALA:HA	2.05	0.57
1:C:228:LEU:O	1:C:231:VAL:HG12	2.05	0.57
1:D:250:LEU:HA	1:D:253:ILE:HG22	1.86	0.57
1:I:250:LEU:HA	1:I:253:ILE:HG22	1.87	0.57
1:J:113:ILE:HA	1:J:114:HIS:HB3	1.86	0.57
1:A:113:ILE:O	1:A:328:ALA:HA	2.03	0.57
1:B:77:ARG:HD3	1:B:416:GLU:CG	2.35	0.57
1:E:113:ILE:HG22	1:E:115:LEU:HD13	1.85	0.57
1:I:113:ILE:HA	1:I:114:HIS:HB3	1.86	0.57
1:H:228:LEU:O	1:H:231:VAL:HG12	2.05	0.57
1:B:205:ALA:N	1:B:206:PRO:HD2	2.20	0.57
1:C:81:VAL:O	1:C:85:ILE:N	2.27	0.57
1:D:113:ILE:HG22	1:D:115:LEU:HD13	1.86	0.57
1:D:205:ALA:N	1:D:206:PRO:HD2	2.20	0.57
1:H:70:ALA:HB1	1:H:163:ILE:HD12	1.85	0.57
1:H:113:ILE:HA	1:H:114:HIS:HB3	1.87	0.57
1:I:70:ALA:HB1	1:I:163:ILE:HD12	1.86	0.57
1:K:205:ALA:N	1:K:206:PRO:HD2	2.20	0.57
1:G:113:ILE:CA	1:G:114:HIS:HB3	2.34	0.57
1:I:334:THR:HB	1:I:337:GLN:HB3	1.87	0.57
1:I:77:ARG:HD3	1:I:416:GLU:CG	2.35	0.56
1:J:349:SER:O	1:J:349:SER:OG	2.22	0.56
1:L:105:ARG:NE	1:L:335:VAL:HG13	2.20	0.56
1:L:228:LEU:O	1:L:231:VAL:HG12	2.05	0.56
1:L:250:LEU:HA	1:L:253:ILE:HG22	1.87	0.56
1:A:113:ILE:HA	1:A:114:HIS:HB3	1.85	0.56
1:B:250:LEU:HA	1:B:253:ILE:HG22	1.87	0.56
1:C:113:ILE:CA	1:C:114:HIS:HB3	2.35	0.56
1:G:334:THR:HB	1:G:337:GLN:HB3	1.86	0.56
1:J:113:ILE:HG22	1:J:115:LEU:HD13	1.85	0.56
1:L:113:ILE:HA	1:L:114:HIS:HB3	1.85	0.56
1:D:113:ILE:HA	1:D:114:HIS:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ILE:O	1:D:328:ALA:HA	2.05	0.56
1:H:77:ARG:HD3	1:H:416:GLU:CG	2.35	0.56
1:H:271:THR:HG22	1:H:281:THR:HG22	1.86	0.56
1:E:334:THR:HB	1:E:337:GLN:HB3	1.88	0.56
1:H:250:LEU:HA	1:H:253:ILE:HG22	1.88	0.56
1:J:334:THR:HB	1:J:337:GLN:HB3	1.88	0.56
1:L:130:LEU:O	1:L:134:LEU:N	2.37	0.56
1:A:155:ILE:HD11	1:A:304:PRO:HB2	1.88	0.56
1:B:70:ALA:HB1	1:B:163:ILE:HD12	1.87	0.56
1:G:105:ARG:NE	1:G:335:VAL:HG13	2.21	0.56
1:I:205:ALA:N	1:I:206:PRO:HD2	2.20	0.56
1:G:113:ILE:HA	1:G:114:HIS:HB3	1.88	0.56
1:G:271:THR:HG22	1:G:281:THR:HG22	1.86	0.56
1:L:70:ALA:HB1	1:L:163:ILE:HD12	1.86	0.56
1:D:105:ARG:NE	1:D:335:VAL:HG13	2.21	0.56
1:G:113:ILE:O	1:G:328:ALA:HA	2.06	0.56
1:G:349:SER:O	1:G:349:SER:OG	2.19	0.56
1:B:113:ILE:HA	1:B:114:HIS:HB3	1.88	0.56
1:D:271:THR:HG22	1:D:281:THR:HG22	1.87	0.56
1:F:228:LEU:O	1:F:231:VAL:HG12	2.06	0.56
1:G:119:GLY:N	1:G:120:GLN:HA	2.21	0.56
1:G:305:LEU:O	1:G:309:ILE:HB	2.05	0.56
1:A:77:ARG:HD3	1:A:416:GLU:HG2	1.89	0.55
1:E:205:ALA:N	1:E:206:PRO:HD2	2.22	0.55
1:C:155:ILE:HD11	1:C:304:PRO:HB2	1.88	0.55
1:F:313:GLY:N	1:F:401:ASN:OD1	2.39	0.55
1:J:105:ARG:NE	1:J:335:VAL:HG13	2.21	0.55
1:C:113:ILE:HA	1:C:114:HIS:HB3	1.89	0.55
1:D:70:ALA:HB1	1:D:163:ILE:HD12	1.89	0.55
1:H:113:ILE:O	1:H:328:ALA:HA	2.06	0.55
1:J:205:ALA:N	1:J:206:PRO:HD2	2.22	0.55
1:K:272:ALA:HA	1:K:281:THR:HG21	1.88	0.55
1:E:117:VAL:HG11	1:E:378:ASN:CB	2.37	0.55
1:K:113:ILE:HA	1:K:114:HIS:HB3	1.89	0.55
1:E:113:ILE:HA	1:E:114:HIS:HB3	1.88	0.55
1:J:250:LEU:HA	1:J:253:ILE:HG22	1.89	0.55
1:H:205:ALA:N	1:H:206:PRO:HD2	2.21	0.55
1:I:113:ILE:O	1:I:328:ALA:HA	2.07	0.55
1:A:250:LEU:HA	1:A:253:ILE:HG22	1.89	0.55
1:B:73:ILE:O	1:B:77:ARG:HB2	2.07	0.55
1:C:250:LEU:HA	1:C:253:ILE:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ARG:HD3	1:E:416:GLU:HG2	1.88	0.55
1:F:105:ARG:NE	1:F:335:VAL:HG13	2.21	0.55
1:I:313:GLY:N	1:I:401:ASN:OD1	2.40	0.55
1:B:105:ARG:NE	1:B:335:VAL:HG13	2.22	0.55
1:I:105:ARG:NE	1:I:335:VAL:HG13	2.22	0.55
1:C:70:ALA:HB1	1:C:163:ILE:HD12	1.89	0.54
1:D:155:ILE:HD11	1:D:304:PRO:HB2	1.88	0.54
1:D:228:LEU:O	1:D:231:VAL:HG12	2.06	0.54
1:E:250:LEU:HA	1:E:253:ILE:HG22	1.90	0.54
1:F:70:ALA:HB1	1:F:163:ILE:HD12	1.89	0.54
1:K:70:ALA:HB1	1:K:163:ILE:HD12	1.89	0.54
1:D:313:GLY:N	1:D:401:ASN:OD1	2.41	0.54
1:F:250:LEU:HA	1:F:253:ILE:HG22	1.89	0.54
1:A:70:ALA:HB1	1:A:163:ILE:HD12	1.88	0.54
1:A:205:ALA:N	1:A:206:PRO:HD2	2.22	0.54
1:H:117:VAL:O	1:H:118:GLY:C	2.50	0.54
1:K:250:LEU:HA	1:K:253:ILE:HG22	1.89	0.54
1:C:205:ALA:N	1:C:206:PRO:HD2	2.23	0.54
1:F:81:VAL:O	1:F:85:ILE:N	2.29	0.54
1:G:155:ILE:HD11	1:G:304:PRO:HB2	1.89	0.54
1:J:70:ALA:HB1	1:J:163:ILE:HD12	1.89	0.54
1:J:228:LEU:O	1:J:231:VAL:HG12	2.08	0.54
1:K:117:VAL:HG11	1:K:378:ASN:CB	2.37	0.54
1:C:113:ILE:HG22	1:C:115:LEU:HD13	1.88	0.54
1:E:113:ILE:O	1:E:328:ALA:HA	2.08	0.54
1:G:250:LEU:HA	1:G:253:ILE:HG22	1.89	0.54
1:F:288:VAL:O	1:F:292:MET:HB2	2.08	0.54
1:I:228:LEU:O	1:I:231:VAL:HG12	2.07	0.54
1:C:73:ILE:HG12	1:I:172:GLU:CB	2.38	0.54
1:H:81:VAL:O	1:H:85:ILE:N	2.29	0.54
1:K:113:ILE:O	1:K:328:ALA:HA	2.07	0.54
1:A:228:LEU:O	1:A:231:VAL:HG12	2.07	0.53
1:D:272:ALA:HA	1:D:281:THR:HG21	1.90	0.53
1:A:73:ILE:O	1:A:77:ARG:HB2	2.08	0.53
1:D:334:THR:HB	1:D:337:GLN:HB3	1.89	0.53
1:F:205:ALA:N	1:F:206:PRO:HD2	2.23	0.53
1:F:234:ALA:HB3	1:F:320:VAL:HG21	1.90	0.53
1:I:255:GLY:O	1:I:256:ILE:C	2.51	0.53
1:J:155:ILE:HD11	1:J:304:PRO:HB2	1.88	0.53
1:B:77:ARG:O	1:B:81:VAL:HG22	2.09	0.53
1:G:70:ALA:HB1	1:G:163:ILE:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:205:ALA:N	1:L:206:PRO:HD2	2.23	0.53
1:C:77:ARG:HD3	1:C:416:GLU:CG	2.39	0.53
1:E:105:ARG:NE	1:E:335:VAL:HG13	2.23	0.53
1:H:234:ALA:HB3	1:H:320:VAL:HG21	1.90	0.53
1:K:105:ARG:NE	1:K:335:VAL:HG13	2.23	0.53
1:E:70:ALA:HB1	1:E:163:ILE:HD12	1.89	0.53
1:F:130:LEU:O	1:F:134:LEU:N	2.35	0.53
1:H:272:ALA:HA	1:H:281:THR:HG21	1.91	0.53
1:J:305:LEU:O	1:J:309:ILE:HB	2.09	0.53
1:A:349:SER:O	1:A:349:SER:OG	2.22	0.53
1:C:271:THR:HG22	1:C:281:THR:HG22	1.89	0.53
1:J:234:ALA:HB3	1:J:320:VAL:HG21	1.91	0.53
1:A:105:ARG:NE	1:A:335:VAL:HG13	2.23	0.53
1:B:117:VAL:O	1:B:118:GLY:C	2.52	0.53
1:G:228:LEU:O	1:G:231:VAL:HG12	2.08	0.53
1:H:255:GLY:O	1:H:256:ILE:C	2.52	0.53
1:K:234:ALA:HB3	1:K:320:VAL:HG21	1.90	0.53
1:H:305:LEU:O	1:H:309:ILE:HB	2.09	0.53
1:J:77:ARG:HD3	1:J:416:GLU:HG2	1.91	0.53
1:K:334:THR:HB	1:K:337:GLN:HB3	1.90	0.53
1:A:299:TYR:CD1	1:A:299:TYR:C	2.87	0.52
1:C:272:ALA:HA	1:C:281:THR:HG21	1.91	0.52
1:D:305:LEU:O	1:D:309:ILE:HB	2.09	0.52
1:F:77:ARG:HD3	1:F:416:GLU:HG2	1.90	0.52
1:D:117:VAL:HG11	1:D:378:ASN:CB	2.39	0.52
1:G:73:ILE:O	1:G:77:ARG:HB2	2.09	0.52
1:G:117:VAL:HG11	1:G:378:ASN:CB	2.39	0.52
1:I:272:ALA:HA	1:I:281:THR:HG21	1.91	0.52
1:G:117:VAL:O	1:G:118:GLY:C	2.52	0.52
1:B:113:ILE:O	1:B:328:ALA:HA	2.09	0.52
1:H:105:ARG:NE	1:H:335:VAL:HG13	2.25	0.52
1:L:313:GLY:N	1:L:401:ASN:OD1	2.41	0.52
1:D:73:ILE:O	1:D:77:ARG:HB2	2.10	0.52
1:L:117:VAL:HG11	1:L:378:ASN:CB	2.40	0.52
1:C:73:ILE:O	1:C:77:ARG:HB2	2.10	0.52
1:D:234:ALA:HB3	1:D:320:VAL:HG21	1.91	0.52
1:L:130:LEU:HD12	1:L:130:LEU:C	2.35	0.52
1:B:272:ALA:HA	1:B:281:THR:HG21	1.92	0.52
1:E:53:LEU:O	1:E:56:MET:HB3	2.09	0.52
1:J:231:VAL:HG23	1:J:320:VAL:HG22	1.92	0.52
1:A:234:ALA:HB3	1:A:320:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:ALA:HB3	1:E:320:VAL:HG21	1.92	0.52
1:J:73:ILE:O	1:J:77:ARG:HB2	2.10	0.52
1:C:117:VAL:HG11	1:C:378:ASN:CB	2.40	0.52
1:C:234:ALA:HB3	1:C:320:VAL:HG21	1.92	0.52
1:F:334:THR:HG22	1:F:337:GLN:HB2	1.92	0.52
1:B:334:THR:HG22	1:B:337:GLN:HB2	1.92	0.51
1:I:73:ILE:O	1:I:77:ARG:HB2	2.10	0.51
1:C:337:GLN:O	1:C:340:THR:OG1	2.28	0.51
1:G:234:ALA:HB3	1:G:320:VAL:HG21	1.92	0.51
1:I:117:VAL:HG11	1:I:378:ASN:CB	2.39	0.51
1:L:334:THR:HG22	1:L:337:GLN:HB2	1.91	0.51
1:B:313:GLY:N	1:B:401:ASN:OD1	2.43	0.51
1:C:305:LEU:O	1:C:309:ILE:HB	2.10	0.51
1:F:117:VAL:O	1:F:118:GLY:C	2.53	0.51
1:G:332:HIS:O	1:G:333:LEU:HD13	2.09	0.51
1:A:117:VAL:O	1:A:118:GLY:C	2.54	0.51
1:E:272:ALA:HA	1:E:281:THR:HG21	1.93	0.51
1:L:231:VAL:HG23	1:L:320:VAL:HG22	1.92	0.51
1:L:288:VAL:O	1:L:292:MET:HB2	2.10	0.51
1:D:198:VAL:O	1:D:202:MET:HG2	2.10	0.51
1:I:234:ALA:HB3	1:I:320:VAL:HG21	1.93	0.51
1:K:117:VAL:O	1:K:118:GLY:C	2.54	0.51
1:K:334:THR:HG22	1:K:337:GLN:HB2	1.93	0.51
1:G:205:ALA:N	1:G:206:PRO:HD2	2.26	0.51
1:J:81:VAL:O	1:J:85:ILE:N	2.32	0.51
1:F:305:LEU:O	1:F:309:ILE:HB	2.11	0.50
1:G:334:THR:HG22	1:G:337:GLN:HB2	1.93	0.50
1:H:231:VAL:HG23	1:H:320:VAL:HG22	1.93	0.50
1:B:80:ARG:O	1:B:82:GLY:N	2.42	0.50
1:F:73:ILE:O	1:F:77:ARG:HB2	2.11	0.50
1:D:152:LEU:N	1:D:153:PRO:CD	2.74	0.50
1:E:117:VAL:O	1:E:118:GLY:C	2.55	0.50
1:H:77:ARG:O	1:H:81:VAL:HG22	2.12	0.50
1:I:198:VAL:O	1:I:202:MET:HG2	2.11	0.50
1:K:77:ARG:HD3	1:K:416:GLU:CG	2.40	0.50
1:L:117:VAL:O	1:L:118:GLY:C	2.53	0.50
1:L:255:GLY:O	1:L:256:ILE:C	2.53	0.50
1:E:130:LEU:O	1:E:134:LEU:N	2.42	0.50
1:J:117:VAL:HG11	1:J:378:ASN:CB	2.40	0.50
1:J:117:VAL:O	1:J:118:GLY:C	2.53	0.50
1:K:299:TYR:CD1	1:K:299:TYR:C	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:HIS:O	1:A:333:LEU:HD13	2.12	0.50
1:D:130:LEU:C	1:D:130:LEU:HD12	2.36	0.50
1:I:334:THR:HG22	1:I:337:GLN:HB2	1.94	0.50
1:D:231:VAL:HG23	1:D:320:VAL:HG22	1.93	0.50
1:J:313:GLY:N	1:J:401:ASN:OD1	2.44	0.50
1:D:332:HIS:O	1:D:333:LEU:HD22	2.12	0.50
1:E:334:THR:HG22	1:E:337:GLN:HB2	1.93	0.50
1:A:313:GLY:N	1:A:401:ASN:OD1	2.45	0.50
1:C:117:VAL:O	1:C:118:GLY:C	2.55	0.50
1:H:8:ILE:O	1:H:8:ILE:HG22	2.12	0.50
1:F:374:LEU:O	1:F:380:ALA:HB2	2.11	0.50
1:G:8:ILE:HG22	1:G:8:ILE:O	2.12	0.50
1:I:117:VAL:O	1:I:118:GLY:C	2.55	0.50
1:I:156:PHE:C	1:I:156:PHE:CD2	2.90	0.50
1:J:80:ARG:O	1:J:82:GLY:N	2.43	0.50
1:K:117:VAL:HG21	1:K:378:ASN:HB2	1.94	0.50
1:A:195:TYR:O	1:A:198:VAL:HG12	2.12	0.49
1:E:77:ARG:O	1:E:81:VAL:HG22	2.12	0.49
1:E:332:HIS:O	1:E:333:LEU:HD13	2.12	0.49
1:H:117:VAL:HG11	1:H:378:ASN:CB	2.42	0.49
1:A:334:THR:HG22	1:A:337:GLN:HB2	1.94	0.49
1:F:117:VAL:HG11	1:F:378:ASN:CB	2.41	0.49
1:G:81:VAL:O	1:G:85:ILE:N	2.29	0.49
1:H:334:THR:HG22	1:H:337:GLN:HB2	1.93	0.49
1:L:234:ALA:HB3	1:L:320:VAL:HG21	1.94	0.49
1:L:272:ALA:HA	1:L:281:THR:HG21	1.94	0.49
1:A:272:ALA:HA	1:A:281:THR:HG21	1.94	0.49
1:K:77:ARG:O	1:K:81:VAL:HG22	2.13	0.49
1:B:231:VAL:HG23	1:B:320:VAL:HG22	1.93	0.49
1:E:231:VAL:HG23	1:E:320:VAL:HG22	1.94	0.49
1:F:255:GLY:O	1:F:256:ILE:C	2.54	0.49
1:I:8:ILE:HG22	1:I:8:ILE:O	2.11	0.49
1:K:192:GLU:O	1:K:193:ALA:C	2.54	0.49
1:C:152:LEU:N	1:C:153:PRO:CD	2.75	0.49
1:D:195:TYR:O	1:D:198:VAL:HG12	2.13	0.49
1:F:272:ALA:HA	1:F:281:THR:HG21	1.94	0.49
1:A:376:ASP:O	1:A:378:ASN:N	2.46	0.49
1:I:231:VAL:HG23	1:I:320:VAL:HG22	1.95	0.49
1:I:255:GLY:O	1:I:256:ILE:O	2.31	0.49
1:L:8:ILE:O	1:L:8:ILE:HG22	2.12	0.49
1:L:81:VAL:O	1:L:85:ILE:N	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:LEU:O	1:D:134:LEU:N	2.41	0.49
1:J:272:ALA:HA	1:J:281:THR:HG21	1.95	0.49
1:A:8:ILE:HG22	1:A:8:ILE:O	2.13	0.49
1:B:305:LEU:O	1:B:309:ILE:HB	2.13	0.49
1:D:337:GLN:O	1:D:340:THR:OG1	2.31	0.49
1:F:376:ASP:O	1:F:378:ASN:N	2.45	0.49
1:L:305:LEU:O	1:L:309:ILE:HB	2.12	0.49
1:F:8:ILE:HG22	1:F:8:ILE:O	2.13	0.49
1:J:8:ILE:O	1:J:8:ILE:HG22	2.13	0.49
1:L:173:ASN:OD1	1:L:174:GLU:N	2.45	0.49
1:B:234:ALA:HB3	1:B:320:VAL:HG21	1.95	0.48
1:C:334:THR:HG22	1:C:337:GLN:HB2	1.94	0.48
1:E:313:GLY:N	1:E:401:ASN:OD1	2.46	0.48
1:H:130:LEU:C	1:H:130:LEU:HD12	2.38	0.48
1:H:313:GLY:N	1:H:401:ASN:OD1	2.45	0.48
1:L:332:HIS:O	1:L:333:LEU:HD13	2.12	0.48
1:L:334:THR:HG22	1:L:337:GLN:CB	2.43	0.48
1:A:77:ARG:O	1:A:81:VAL:HG22	2.13	0.48
1:D:413:ALA:C	1:D:415:THR:H	2.21	0.48
1:E:59:MET:HB2	1:E:60:PRO:HD3	1.95	0.48
1:F:231:VAL:HG23	1:F:320:VAL:HG22	1.93	0.48
1:F:339:LEU:HD13	1:F:340:THR:H	1.78	0.48
1:G:255:GLY:O	1:G:256:ILE:C	2.55	0.48
1:A:255:GLY:O	1:A:256:ILE:C	2.56	0.48
1:A:374:LEU:O	1:A:380:ALA:HB2	2.12	0.48
1:B:332:HIS:O	1:B:333:LEU:HD13	2.13	0.48
1:E:8:ILE:O	1:E:8:ILE:HG22	2.13	0.48
1:F:332:HIS:O	1:F:333:LEU:HD22	2.13	0.48
1:F:334:THR:HG22	1:F:337:GLN:CB	2.43	0.48
1:H:413:ALA:C	1:H:415:THR:H	2.21	0.48
1:I:173:ASN:OD1	1:I:174:GLU:N	2.47	0.48
1:J:299:TYR:CD1	1:J:299:TYR:C	2.91	0.48
1:L:376:ASP:O	1:L:378:ASN:N	2.47	0.48
1:A:160:ILE:CG2	1:C:197:ILE:HD12	2.44	0.48
1:B:299:TYR:CD1	1:B:299:TYR:C	2.91	0.48
1:E:156:PHE:C	1:E:156:PHE:CD2	2.92	0.48
1:A:152:LEU:N	1:A:153:PRO:CD	2.77	0.48
1:A:231:VAL:HG23	1:A:320:VAL:HG22	1.95	0.48
1:G:272:ALA:HA	1:G:281:THR:HG21	1.94	0.48
1:H:332:HIS:O	1:H:333:LEU:HD22	2.13	0.48
1:K:119:GLY:N	1:K:120:GLN:HA	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:HD12	1:B:130:LEU:C	2.38	0.48
1:G:231:VAL:HG23	1:G:320:VAL:HG22	1.95	0.48
1:I:84:LYS:O	1:I:88:TYR:N	2.46	0.48
1:J:130:LEU:O	1:J:134:LEU:N	2.39	0.48
1:J:374:LEU:O	1:J:380:ALA:HB2	2.14	0.48
1:L:77:ARG:O	1:L:81:VAL:HG22	2.13	0.48
1:H:119:GLY:N	1:H:120:GLN:HA	2.28	0.48
1:J:255:GLY:O	1:J:256:ILE:C	2.56	0.48
1:B:334:THR:HG22	1:B:337:GLN:CB	2.44	0.48
1:I:81:VAL:O	1:I:85:ILE:N	2.34	0.48
1:J:334:THR:HG22	1:J:337:GLN:HB2	1.96	0.48
1:K:231:VAL:HG23	1:K:320:VAL:HG22	1.95	0.48
1:C:173:ASN:OD1	1:C:174:GLU:N	2.46	0.48
1:E:73:ILE:O	1:E:77:ARG:HB2	2.13	0.48
1:G:130:LEU:HD12	1:G:130:LEU:C	2.38	0.48
1:G:197:ILE:HD12	1:H:160:ILE:CG2	2.44	0.48
1:B:117:VAL:HG11	1:B:378:ASN:CB	2.40	0.48
1:C:8:ILE:O	1:C:8:ILE:HG22	2.14	0.48
1:E:334:THR:HG22	1:E:337:GLN:CB	2.44	0.48
1:K:255:GLY:O	1:K:256:ILE:C	2.57	0.48
1:L:339:LEU:HD13	1:L:340:THR:H	1.78	0.48
1:D:255:GLY:O	1:D:256:ILE:C	2.57	0.47
1:E:192:GLU:O	1:E:193:ALA:C	2.57	0.47
1:I:413:ALA:C	1:I:415:THR:H	2.22	0.47
1:J:156:PHE:C	1:J:156:PHE:CD2	2.92	0.47
1:J:332:HIS:O	1:J:333:LEU:HD13	2.14	0.47
1:A:173:ASN:OD1	1:A:174:GLU:N	2.48	0.47
1:C:231:VAL:HG23	1:C:320:VAL:HG22	1.96	0.47
1:C:332:HIS:O	1:C:333:LEU:HD22	2.14	0.47
1:K:73:ILE:O	1:K:77:ARG:HB2	2.14	0.47
1:B:8:ILE:HG22	1:B:8:ILE:O	2.14	0.47
1:C:413:ALA:C	1:C:415:THR:H	2.22	0.47
1:J:332:HIS:O	1:J:333:LEU:HD22	2.14	0.47
1:A:198:VAL:O	1:A:202:MET:HG2	2.13	0.47
1:D:117:VAL:O	1:D:118:GLY:C	2.57	0.47
1:F:173:ASN:OD1	1:F:174:GLU:N	2.48	0.47
1:J:130:LEU:HD12	1:J:130:LEU:C	2.39	0.47
1:K:334:THR:HG22	1:K:337:GLN:CB	2.44	0.47
1:A:117:VAL:HG11	1:A:378:ASN:CB	2.43	0.47
1:C:73:ILE:O	1:C:76:ALA:O	2.32	0.47
1:D:339:LEU:HD13	1:D:340:THR:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:LEU:HD13	1:E:340:THR:H	1.80	0.47
1:H:334:THR:HG22	1:H:337:GLN:CB	2.44	0.47
1:I:152:LEU:N	1:I:153:PRO:CD	2.78	0.47
1:E:299:TYR:CD1	1:E:299:TYR:C	2.91	0.47
1:E:305:LEU:O	1:E:309:ILE:HB	2.13	0.47
1:F:130:LEU:C	1:F:130:LEU:HD12	2.38	0.47
1:G:173:ASN:OD1	1:G:174:GLU:N	2.48	0.47
1:K:8:ILE:HG22	1:K:8:ILE:O	2.15	0.47
1:A:332:HIS:O	1:A:333:LEU:HD22	2.15	0.47
1:D:8:ILE:HG22	1:D:8:ILE:O	2.14	0.47
1:D:299:TYR:CD1	1:D:299:TYR:C	2.92	0.47
1:F:299:TYR:CD1	1:F:299:TYR:C	2.92	0.47
1:G:275:THR:HG22	1:G:277:SER:HB3	1.97	0.47
1:H:152:LEU:N	1:H:153:PRO:CD	2.78	0.47
1:K:173:ASN:OD1	1:K:174:GLU:N	2.48	0.47
1:K:339:LEU:HD13	1:K:340:THR:H	1.80	0.47
1:C:339:LEU:HD13	1:C:340:THR:H	1.80	0.47
1:C:376:ASP:O	1:C:378:ASN:N	2.48	0.47
1:E:130:LEU:HD12	1:E:130:LEU:C	2.40	0.47
1:E:332:HIS:O	1:E:333:LEU:HD22	2.15	0.47
1:E:374:LEU:O	1:E:380:ALA:HB2	2.15	0.47
1:G:77:ARG:O	1:G:81:VAL:HG22	2.15	0.47
1:G:339:LEU:HD13	1:G:340:THR:H	1.80	0.47
1:H:332:HIS:O	1:H:333:LEU:HD13	2.14	0.47
1:I:77:ARG:O	1:I:81:VAL:HG22	2.14	0.47
1:I:117:VAL:HG21	1:I:378:ASN:HB2	1.97	0.47
1:J:117:VAL:HG21	1:J:378:ASN:HB2	1.97	0.47
1:B:192:GLU:O	1:B:193:ALA:C	2.57	0.47
1:B:339:LEU:HD13	1:B:340:THR:H	1.80	0.47
1:D:156:PHE:C	1:D:156:PHE:CD2	2.93	0.47
1:H:323:PHE:CE1	1:H:333:LEU:HD11	2.50	0.47
1:K:152:LEU:N	1:K:153:PRO:CD	2.78	0.47
1:B:255:GLY:O	1:B:256:ILE:C	2.57	0.47
1:D:334:THR:HG22	1:D:337:GLN:HB2	1.97	0.47
1:F:117:VAL:HG21	1:F:378:ASN:HB2	1.97	0.47
1:I:374:LEU:O	1:I:380:ALA:HB2	2.15	0.47
1:J:119:GLY:N	1:J:120:GLN:HA	2.30	0.47
1:K:332:HIS:O	1:K:333:LEU:HD13	2.16	0.46
1:L:339:LEU:O	1:L:340:THR:C	2.58	0.46
1:A:130:LEU:O	1:A:134:LEU:N	2.40	0.46
1:C:130:LEU:C	1:C:130:LEU:HD12	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:LYS:HG3	1:E:176:VAL:N	2.30	0.46
1:L:198:VAL:O	1:L:202:MET:HG2	2.15	0.46
1:A:305:LEU:O	1:A:309:ILE:HB	2.16	0.46
1:B:156:PHE:C	1:B:156:PHE:CD2	2.93	0.46
1:F:294:ILE:HG22	1:F:295:SER:N	2.31	0.46
1:H:173:ASN:OD1	1:H:174:GLU:N	2.48	0.46
1:H:337:GLN:O	1:H:340:THR:OG1	2.34	0.46
1:D:173:ASN:OD1	1:D:174:GLU:N	2.49	0.46
1:G:376:ASP:O	1:G:378:ASN:N	2.49	0.46
1:H:198:VAL:O	1:H:202:MET:HG2	2.16	0.46
1:I:130:LEU:O	1:I:134:LEU:N	2.41	0.46
1:A:337:GLN:O	1:A:340:THR:OG1	2.34	0.46
1:D:117:VAL:HG21	1:D:378:ASN:HB2	1.98	0.46
1:F:195:TYR:O	1:F:198:VAL:HG12	2.15	0.46
1:G:332:HIS:O	1:G:333:LEU:HD22	2.15	0.46
1:D:81:VAL:O	1:D:85:ILE:N	2.31	0.46
1:I:332:HIS:O	1:I:333:LEU:HD22	2.15	0.46
1:J:105:ARG:CZ	1:J:335:VAL:HG13	2.46	0.46
1:K:332:HIS:O	1:K:333:LEU:HD22	2.14	0.46
1:E:81:VAL:O	1:E:85:ILE:N	2.33	0.46
1:F:332:HIS:O	1:F:333:LEU:HD13	2.16	0.46
1:G:334:THR:HG22	1:G:337:GLN:CB	2.45	0.46
1:H:299:TYR:CD1	1:H:299:TYR:C	2.94	0.46
1:J:357:GLY:O	1:J:361:ILE:HD13	2.16	0.46
1:A:160:ILE:HG23	1:C:197:ILE:HD12	1.98	0.46
1:A:334:THR:HG22	1:A:337:GLN:CB	2.46	0.46
1:C:105:ARG:CZ	1:C:335:VAL:HG13	2.45	0.46
1:I:305:LEU:O	1:I:309:ILE:HB	2.16	0.46
1:I:337:GLN:O	1:I:340:THR:OG1	2.33	0.46
1:J:323:PHE:CE1	1:J:333:LEU:HD11	2.51	0.46
1:C:77:ARG:O	1:C:81:VAL:HG22	2.15	0.46
1:I:73:ILE:O	1:I:76:ALA:O	2.34	0.46
1:I:175:LYS:HG3	1:I:176:VAL:N	2.31	0.46
1:K:376:ASP:O	1:K:379:VAL:N	2.49	0.46
1:L:334:THR:CG2	1:L:337:GLN:HB3	2.46	0.46
1:A:156:PHE:CD2	1:A:156:PHE:C	2.93	0.46
1:C:334:THR:HG22	1:C:337:GLN:CB	2.46	0.46
1:I:334:THR:HG22	1:I:337:GLN:CB	2.46	0.46
1:J:337:GLN:O	1:J:340:THR:OG1	2.33	0.46
1:A:413:ALA:C	1:A:415:THR:H	2.24	0.45
1:D:198:VAL:CG1	1:D:287:ARG:HD3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:60:PRO:HB2	1:I:194:MET:HG3	1.98	0.45
1:J:195:TYR:O	1:J:198:VAL:HG12	2.16	0.45
1:L:105:ARG:CZ	1:L:335:VAL:HG13	2.46	0.45
1:B:337:GLN:O	1:B:340:THR:OG1	2.34	0.45
1:E:413:ALA:C	1:E:415:THR:H	2.24	0.45
1:F:44:LYS:HB3	1:F:45:PRO:HD3	1.98	0.45
1:G:105:ARG:CZ	1:G:335:VAL:HG13	2.47	0.45
1:H:73:ILE:O	1:H:77:ARG:HB2	2.16	0.45
1:H:156:PHE:C	1:H:156:PHE:CD2	2.93	0.45
1:K:175:LYS:HG3	1:K:176:VAL:N	2.30	0.45
1:A:391:ALA:O	1:A:395:MET:HG3	2.16	0.45
1:C:332:HIS:O	1:C:333:LEU:HD13	2.15	0.45
1:I:303:LEU:HB2	1:I:304:PRO:HD3	1.96	0.45
1:J:376:ASP:O	1:J:378:ASN:N	2.49	0.45
1:K:130:LEU:O	1:K:134:LEU:N	2.43	0.45
1:K:197:ILE:HD12	1:L:160:ILE:CG2	2.46	0.45
1:L:152:LEU:N	1:L:153:PRO:CD	2.79	0.45
1:L:332:HIS:O	1:L:333:LEU:HD22	2.16	0.45
1:C:255:GLY:O	1:C:256:ILE:C	2.59	0.45
1:F:213:ILE:HD12	1:F:213:ILE:C	2.42	0.45
1:G:44:LYS:HB3	1:G:45:PRO:HD3	1.98	0.45
1:H:376:ASP:O	1:H:378:ASN:N	2.49	0.45
1:I:213:ILE:C	1:I:213:ILE:HD12	2.41	0.45
1:I:323:PHE:CE1	1:I:333:LEU:HD11	2.52	0.45
1:K:81:VAL:O	1:K:85:ILE:N	2.33	0.45
1:K:239:LEU:HB2	1:K:400:VAL:HG21	1.99	0.45
1:B:105:ARG:CZ	1:B:335:VAL:HG13	2.46	0.45
1:F:77:ARG:O	1:F:81:VAL:HG22	2.15	0.45
1:F:413:ALA:C	1:F:415:THR:H	2.25	0.45
1:G:197:ILE:HD12	1:H:160:ILE:HG23	1.99	0.45
1:G:337:GLN:O	1:G:340:THR:OG1	2.34	0.45
1:H:195:TYR:O	1:H:198:VAL:HG12	2.17	0.45
1:K:130:LEU:C	1:K:130:LEU:HD12	2.41	0.45
1:K:305:LEU:O	1:K:309:ILE:HB	2.16	0.45
1:B:117:VAL:HG21	1:B:378:ASN:HB2	1.99	0.45
1:G:374:LEU:O	1:G:380:ALA:HB2	2.17	0.45
1:H:130:LEU:O	1:H:134:LEU:N	2.42	0.45
1:L:299:TYR:CD1	1:L:299:TYR:C	2.94	0.45
1:L:334:THR:CB	1:L:337:GLN:HB3	2.46	0.45
1:A:44:LYS:HB3	1:A:45:PRO:HD3	1.98	0.45
1:B:173:ASN:OD1	1:B:174:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:VAL:HG21	1:E:378:ASN:HB2	1.98	0.45
1:E:173:ASN:OD1	1:E:174:GLU:N	2.50	0.45
1:H:334:THR:CG2	1:H:337:GLN:HB3	2.47	0.45
1:J:198:VAL:O	1:J:202:MET:HG2	2.17	0.45
1:J:339:LEU:HD13	1:J:340:THR:H	1.81	0.45
1:K:195:TYR:O	1:K:198:VAL:HG12	2.16	0.45
1:L:73:ILE:O	1:L:77:ARG:HB2	2.17	0.45
1:C:334:THR:O	1:C:337:GLN:N	2.44	0.45
1:F:119:GLY:N	1:F:120:GLN:HA	2.31	0.45
1:J:73:ILE:O	1:J:76:ALA:O	2.34	0.45
1:K:376:ASP:O	1:K:378:ASN:N	2.50	0.45
1:B:334:THR:CG2	1:B:337:GLN:HB3	2.47	0.45
1:F:334:THR:CG2	1:F:337:GLN:HB3	2.46	0.45
1:K:105:ARG:CZ	1:K:335:VAL:HG13	2.47	0.45
1:A:117:VAL:HG21	1:A:378:ASN:HB2	2.00	0.45
1:B:198:VAL:O	1:B:202:MET:HG2	2.17	0.45
1:C:198:VAL:O	1:C:202:MET:HG2	2.17	0.45
1:C:313:GLY:N	1:C:401:ASN:OD1	2.50	0.45
1:E:152:LEU:N	1:E:153:PRO:CD	2.80	0.45
1:G:160:ILE:CG2	1:I:197:ILE:HD12	2.47	0.45
1:I:339:LEU:HD13	1:I:340:THR:H	1.82	0.45
1:K:59:MET:HB2	1:K:60:PRO:HD3	1.99	0.45
1:L:303:LEU:HB2	1:L:304:PRO:HD3	1.99	0.45
1:C:117:VAL:HG21	1:C:378:ASN:HB2	1.98	0.44
1:C:323:PHE:CE1	1:C:333:LEU:HD11	2.52	0.44
1:E:255:GLY:O	1:E:256:ILE:C	2.60	0.44
1:G:105:ARG:HH21	1:G:338:GLN:NE2	2.15	0.44
1:I:105:ARG:CZ	1:I:335:VAL:HG13	2.47	0.44
1:J:173:ASN:OD1	1:J:174:GLU:N	2.50	0.44
1:K:53:LEU:O	1:K:56:MET:HB3	2.16	0.44
1:L:334:THR:CG2	1:L:337:GLN:CB	2.95	0.44
1:D:215:TYR:CE1	1:D:219:GLU:HG3	2.52	0.44
1:G:198:VAL:O	1:G:202:MET:HG2	2.16	0.44
1:L:323:PHE:CE1	1:L:333:LEU:HD11	2.53	0.44
1:B:73:ILE:O	1:B:76:ALA:O	2.35	0.44
1:B:374:LEU:O	1:B:380:ALA:HB2	2.17	0.44
1:D:303:LEU:HB2	1:D:304:PRO:HD3	1.98	0.44
1:H:357:GLY:O	1:H:361:ILE:HD13	2.17	0.44
1:I:191:ALA:O	1:I:195:TYR:CD1	2.71	0.44
1:A:130:LEU:C	1:A:130:LEU:HD12	2.41	0.44
1:B:303:LEU:HB2	1:B:304:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:ILE:CG2	1:F:102:ILE:O	2.65	0.44
1:F:323:PHE:CE1	1:F:333:LEU:HD11	2.53	0.44
1:G:63:PHE:O	1:G:67:VAL:HG23	2.16	0.44
1:J:413:ALA:C	1:J:415:THR:H	2.26	0.44
1:K:413:ALA:C	1:K:415:THR:H	2.25	0.44
1:L:105:ARG:HH21	1:L:338:GLN:NE2	2.15	0.44
1:L:301:PHE:O	1:L:301:PHE:CG	2.70	0.44
1:L:374:LEU:O	1:L:380:ALA:HB2	2.16	0.44
1:B:323:PHE:CE1	1:B:333:LEU:HD11	2.53	0.44
1:D:59:MET:HB2	1:D:60:PRO:HD3	2.00	0.44
1:D:105:ARG:CZ	1:D:335:VAL:HG13	2.47	0.44
1:D:332:HIS:O	1:D:333:LEU:HD13	2.17	0.44
1:K:374:LEU:O	1:K:380:ALA:HB2	2.18	0.44
1:B:152:LEU:N	1:B:153:PRO:CD	2.81	0.44
1:C:376:ASP:O	1:C:379:VAL:N	2.51	0.44
1:D:77:ARG:O	1:D:81:VAL:HG22	2.18	0.44
1:D:192:GLU:O	1:D:193:ALA:C	2.60	0.44
1:F:105:ARG:HH22	1:F:338:GLN:HB2	1.82	0.44
1:G:59:MET:HB2	1:G:60:PRO:HD3	2.00	0.44
1:L:198:VAL:CG1	1:L:287:ARG:HD3	2.48	0.44
1:A:197:ILE:HD12	1:B:160:ILE:CG2	2.48	0.44
1:B:332:HIS:O	1:B:333:LEU:HD22	2.17	0.44
1:D:374:LEU:O	1:D:380:ALA:HB2	2.17	0.44
1:E:376:ASP:O	1:E:378:ASN:N	2.51	0.44
1:L:117:VAL:HG21	1:L:378:ASN:HB2	2.00	0.44
1:C:190:LEU:O	1:C:191:ALA:C	2.61	0.44
1:F:152:LEU:N	1:F:153:PRO:CD	2.81	0.44
1:J:152:LEU:N	1:J:153:PRO:CD	2.81	0.44
1:A:73:ILE:O	1:A:76:ALA:O	2.35	0.44
1:B:60:PRO:HB2	1:B:194:MET:HG3	1.98	0.44
1:F:334:THR:CG2	1:F:337:GLN:CB	2.96	0.44
1:G:130:LEU:O	1:G:134:LEU:N	2.41	0.44
1:J:303:LEU:HB2	1:J:304:PRO:HD3	1.99	0.44
1:B:59:MET:HB2	1:B:60:PRO:HD3	2.00	0.43
1:B:334:THR:O	1:B:337:GLN:N	2.43	0.43
1:C:303:LEU:HB2	1:C:304:PRO:HD3	2.00	0.43
1:E:303:LEU:HB2	1:E:304:PRO:HD3	2.00	0.43
1:G:323:PHE:CE1	1:G:333:LEU:HD11	2.53	0.43
1:I:130:LEU:C	1:I:130:LEU:HD12	2.43	0.43
1:J:334:THR:HG22	1:J:337:GLN:CB	2.48	0.43
1:A:59:MET:HB2	1:A:60:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ILE:HG22	1:B:295:SER:N	2.33	0.43
1:E:105:ARG:CZ	1:E:335:VAL:HG13	2.47	0.43
1:F:105:ARG:CZ	1:F:335:VAL:HG13	2.47	0.43
1:H:282:LEU:HD21	1:H:304:PRO:HA	1.99	0.43
1:H:334:THR:CB	1:H:337:GLN:HB3	2.48	0.43
1:K:198:VAL:O	1:K:202:MET:HG2	2.18	0.43
1:B:334:THR:CB	1:B:337:GLN:HB3	2.48	0.43
1:B:413:ALA:C	1:B:415:THR:H	2.25	0.43
1:C:145:ALA:HA	1:C:150:GLN:NE2	2.32	0.43
1:F:197:ILE:H	1:F:197:ILE:HG12	1.71	0.43
1:F:198:VAL:O	1:F:202:MET:HG2	2.18	0.43
1:G:299:TYR:CD1	1:G:299:TYR:C	2.96	0.43
1:I:79:GLY:O	1:I:83:VAL:HG23	2.18	0.43
1:K:197:ILE:HD12	1:L:160:ILE:HG23	2.00	0.43
1:B:105:ARG:HH22	1:B:336:GLY:H	1.65	0.43
1:C:374:LEU:O	1:C:380:ALA:HB2	2.18	0.43
1:D:105:ARG:HH22	1:D:338:GLN:HB2	1.82	0.43
1:F:319:GLY:O	1:F:322:THR:HG22	2.18	0.43
1:G:60:PRO:HB2	1:G:194:MET:HG3	1.99	0.43
1:G:77:ARG:HD3	1:G:416:GLU:CG	2.48	0.43
1:G:413:ALA:C	1:G:415:THR:H	2.26	0.43
1:K:105:ARG:HH21	1:K:338:GLN:NE2	2.16	0.43
1:K:190:LEU:O	1:K:191:ALA:C	2.61	0.43
1:L:413:ALA:C	1:L:415:THR:H	2.26	0.43
1:A:105:ARG:HH21	1:A:338:GLN:NE2	2.16	0.43
1:A:339:LEU:HD13	1:A:340:THR:H	1.83	0.43
1:D:282:LEU:HD21	1:D:304:PRO:HA	2.01	0.43
1:E:105:ARG:HH22	1:E:338:GLN:HB2	1.82	0.43
1:F:303:LEU:HB2	1:F:304:PRO:HD3	2.00	0.43
1:G:152:LEU:N	1:G:153:PRO:CD	2.81	0.43
1:H:374:LEU:O	1:H:380:ALA:HB2	2.18	0.43
1:L:44:LYS:HB3	1:L:45:PRO:HD3	1.99	0.43
1:B:175:LYS:HG3	1:B:176:VAL:N	2.34	0.43
1:C:192:GLU:O	1:C:193:ALA:C	2.62	0.43
1:F:334:THR:O	1:F:337:GLN:N	2.45	0.43
1:F:339:LEU:O	1:F:340:THR:C	2.62	0.43
1:G:117:VAL:HG21	1:G:378:ASN:HB2	1.99	0.43
1:G:303:LEU:HB2	1:G:304:PRO:HD3	2.01	0.43
1:I:299:TYR:C	1:I:299:TYR:CD1	2.97	0.43
1:L:215:TYR:CE1	1:L:219:GLU:HG3	2.53	0.43
1:B:376:ASP:HA	1:B:377:PRO:HD3	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:VAL:O	1:E:202:MET:HG2	2.17	0.43
1:H:255:GLY:O	1:H:256:ILE:O	2.36	0.43
1:I:113:ILE:HD13	1:I:113:ILE:N	2.33	0.43
1:J:105:ARG:HH21	1:J:338:GLN:NE2	2.16	0.43
1:B:334:THR:CG2	1:B:337:GLN:CB	2.96	0.43
1:D:213:ILE:C	1:D:213:ILE:HD12	2.43	0.43
1:D:323:PHE:CE1	1:D:333:LEU:HD11	2.53	0.43
1:H:105:ARG:CZ	1:H:335:VAL:HG13	2.49	0.43
1:H:117:VAL:HG21	1:H:378:ASN:HB2	2.01	0.43
1:H:334:THR:CG2	1:H:337:GLN:CB	2.96	0.43
1:A:175:LYS:HG3	1:A:176:VAL:N	2.34	0.43
1:A:334:THR:CG2	1:A:337:GLN:HB3	2.49	0.43
1:C:44:LYS:HB3	1:C:45:PRO:HD3	1.99	0.43
1:D:334:THR:HG22	1:D:337:GLN:CB	2.48	0.43
1:F:73:ILE:O	1:F:76:ALA:O	2.36	0.43
1:G:159:ILE:HD11	1:G:301:PHE:CD1	2.54	0.43
1:B:376:ASP:O	1:B:378:ASN:N	2.51	0.43
1:D:105:ARG:HH21	1:D:338:GLN:NE2	2.17	0.43
1:G:105:ARG:HH22	1:G:338:GLN:HB2	1.82	0.43
1:H:73:ILE:O	1:H:76:ALA:O	2.37	0.43
1:H:303:LEU:HB2	1:H:304:PRO:HD3	2.01	0.43
1:K:313:GLY:N	1:K:401:ASN:OD1	2.49	0.43
1:A:105:ARG:CZ	1:A:335:VAL:HG13	2.48	0.42
1:A:323:PHE:CE1	1:A:333:LEU:HD11	2.54	0.42
1:D:44:LYS:HB3	1:D:45:PRO:HD3	2.01	0.42
1:D:376:ASP:O	1:D:378:ASN:N	2.52	0.42
1:E:55:LYS:O	1:E:56:MET:C	2.62	0.42
1:E:105:ARG:HH21	1:E:338:GLN:NE2	2.16	0.42
1:F:59:MET:HB2	1:F:60:PRO:HD3	2.01	0.42
1:F:105:ARG:HH21	1:F:338:GLN:NE2	2.17	0.42
1:G:156:PHE:CD2	1:G:156:PHE:C	2.96	0.42
1:H:339:LEU:HD13	1:H:340:THR:H	1.83	0.42
1:J:213:ILE:C	1:J:213:ILE:HD12	2.43	0.42
1:K:156:PHE:CD2	1:K:156:PHE:C	2.97	0.42
1:K:303:LEU:HB2	1:K:304:PRO:HD3	2.01	0.42
1:A:303:LEU:HB2	1:A:304:PRO:HD3	2.00	0.42
1:F:179:SER:O	1:F:180:ALA:C	2.62	0.42
1:H:59:MET:HB2	1:H:60:PRO:HD3	2.00	0.42
1:I:105:ARG:HH22	1:I:338:GLN:HB2	1.82	0.42
1:K:105:ARG:HH22	1:K:338:GLN:HB2	1.83	0.42
1:C:376:ASP:HA	1:C:377:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:GLY:O	1:D:83:VAL:HG23	2.19	0.42
1:H:79:GLY:O	1:H:83:VAL:HG23	2.20	0.42
1:I:282:LEU:HD21	1:I:304:PRO:HA	2.00	0.42
1:I:332:HIS:O	1:I:333:LEU:HD13	2.18	0.42
1:K:323:PHE:CE1	1:K:333:LEU:HD11	2.55	0.42
1:L:73:ILE:O	1:L:76:ALA:O	2.37	0.42
1:A:60:PRO:HB2	1:A:194:MET:HG3	2.01	0.42
1:B:113:ILE:HD13	1:B:113:ILE:N	2.35	0.42
1:C:105:ARG:HH21	1:C:338:GLN:NE2	2.17	0.42
1:C:275:THR:HG22	1:C:277:SER:HB3	2.00	0.42
1:E:44:LYS:HB3	1:E:45:PRO:HD3	2.01	0.42
1:E:197:ILE:H	1:E:197:ILE:HG12	1.74	0.42
1:E:275:THR:HG22	1:E:277:SER:HB3	2.02	0.42
1:E:337:GLN:O	1:E:340:THR:OG1	2.37	0.42
1:G:88:TYR:CZ	1:G:92:THR:HG21	2.54	0.42
1:G:144:GLY:O	1:G:145:ALA:C	2.62	0.42
1:H:197:ILE:HD13	1:I:164:ALA:HB2	2.01	0.42
1:J:59:MET:HB2	1:J:60:PRO:HD3	2.00	0.42
1:K:213:ILE:HD12	1:K:213:ILE:C	2.44	0.42
1:A:9:GLU:OE1	1:A:10:TYR:CE2	2.73	0.42
1:A:48:ASP:O	1:A:51:VAL:N	2.52	0.42
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.54	0.42
1:A:282:LEU:HD21	1:A:304:PRO:HA	2.01	0.42
1:B:81:VAL:O	1:B:85:ILE:N	2.35	0.42
1:B:213:ILE:C	1:B:213:ILE:HD12	2.44	0.42
1:C:209:VAL:HA	1:C:274:VAL:HG11	2.02	0.42
1:E:269:MET:O	1:E:399:MET:HG3	2.20	0.42
1:F:255:GLY:O	1:F:256:ILE:O	2.38	0.42
1:F:334:THR:CB	1:F:337:GLN:HB3	2.48	0.42
1:I:215:TYR:CE1	1:I:219:GLU:HG3	2.54	0.42
1:J:210:PHE:O	1:J:214:ALA:HB2	2.20	0.42
1:L:269:MET:O	1:L:399:MET:HG3	2.20	0.42
1:A:80:ARG:O	1:A:82:GLY:N	2.48	0.42
1:A:192:GLU:O	1:A:193:ALA:C	2.62	0.42
1:B:328:ALA:C	1:B:330:GLY:H	2.27	0.42
1:C:80:ARG:HD2	1:C:80:ARG:HA	1.93	0.42
1:C:127:ALA:N	1:C:128:PRO:CD	2.82	0.42
1:D:105:ARG:HH22	1:D:336:GLY:H	1.67	0.42
1:D:197:ILE:H	1:D:197:ILE:HG12	1.72	0.42
1:E:317:TYR:O	1:E:321:CYS:HB2	2.19	0.42
1:G:175:LYS:HG3	1:G:176:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179:SER:O	1:H:180:ALA:C	2.63	0.42
1:I:59:MET:HB2	1:I:60:PRO:HD3	2.01	0.42
1:K:282:LEU:HD21	1:K:304:PRO:HA	2.01	0.42
1:C:105:ARG:HH22	1:C:338:GLN:HB2	1.83	0.42
1:C:213:ILE:HD12	1:C:213:ILE:C	2.44	0.42
1:G:79:GLY:O	1:G:83:VAL:HG23	2.20	0.42
1:I:159:ILE:HD11	1:I:301:PHE:CD1	2.54	0.42
1:K:334:THR:CG2	1:K:337:GLN:HB3	2.49	0.42
1:L:156:PHE:CD2	1:L:156:PHE:C	2.96	0.42
1:L:255:GLY:O	1:L:256:ILE:O	2.37	0.42
1:A:81:VAL:O	1:A:85:ILE:N	2.33	0.42
1:I:9:GLU:O	1:I:10:TYR:HB2	2.20	0.42
1:J:105:ARG:HH22	1:J:338:GLN:HB2	1.84	0.42
1:C:105:ARG:CZ	1:C:335:VAL:CG1	2.98	0.42
1:D:73:ILE:O	1:D:76:ALA:O	2.37	0.42
1:D:319:GLY:O	1:D:322:THR:HG22	2.20	0.42
1:E:376:ASP:O	1:E:379:VAL:N	2.52	0.42
1:F:81:VAL:HA	1:F:84:LYS:HB2	2.01	0.42
1:H:88:TYR:CZ	1:H:92:THR:HG21	2.55	0.42
1:I:357:GLY:O	1:I:361:ILE:HD13	2.20	0.42
1:I:391:ALA:O	1:I:395:MET:HG3	2.20	0.42
1:J:77:ARG:O	1:J:81:VAL:HG22	2.19	0.42
1:J:275:THR:HG22	1:J:277:SER:HB3	2.01	0.42
1:K:105:ARG:HH22	1:K:336:GLY:H	1.68	0.42
1:L:105:ARG:HH22	1:L:338:GLN:HB2	1.82	0.42
1:A:79:GLY:O	1:A:83:VAL:HG23	2.20	0.42
1:A:275:THR:HG22	1:A:277:SER:HB3	2.01	0.42
1:C:63:PHE:O	1:C:67:VAL:HG23	2.20	0.42
1:D:144:GLY:O	1:D:145:ALA:C	2.62	0.42
1:E:323:PHE:CE1	1:E:333:LEU:HD11	2.54	0.42
1:G:23:GLY:HA2	1:G:26:VAL:HG12	2.02	0.42
1:J:88:TYR:CZ	1:J:92:THR:HG21	2.55	0.42
1:K:337:GLN:O	1:K:340:THR:OG1	2.38	0.42
1:B:79:GLY:O	1:B:83:VAL:HG23	2.20	0.41
1:B:130:LEU:O	1:B:134:LEU:N	2.42	0.41
1:C:137:ILE:O	1:C:153:PRO:HA	2.20	0.41
1:F:175:LYS:HG3	1:F:176:VAL:N	2.34	0.41
1:I:376:ASP:O	1:I:378:ASN:N	2.52	0.41
1:J:80:ARG:HD2	1:J:80:ARG:HA	1.93	0.41
1:L:197:ILE:H	1:L:197:ILE:HG12	1.71	0.41
1:A:334:THR:O	1:A:337:GLN:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ARG:HH21	1:B:338:GLN:NE2	2.17	0.41
1:D:9:GLU:O	1:D:10:TYR:HB2	2.21	0.41
1:D:157:PHE:HD1	1:F:56:MET:HE3	1.85	0.41
1:D:339:LEU:O	1:D:340:THR:C	2.63	0.41
1:E:195:TYR:O	1:E:198:VAL:HG12	2.20	0.41
1:E:282:LEU:HD21	1:E:304:PRO:HA	2.01	0.41
1:E:334:THR:CG2	1:E:337:GLN:CB	2.98	0.41
1:L:59:MET:HB2	1:L:60:PRO:HD3	2.01	0.41
1:A:235:VAL:HG23	1:A:320:VAL:HG11	2.03	0.41
1:A:334:THR:CG2	1:A:337:GLN:CB	2.98	0.41
1:B:215:TYR:CE1	1:B:219:GLU:HG3	2.55	0.41
1:C:113:ILE:N	1:C:113:ILE:HD13	2.35	0.41
1:E:239:LEU:HB2	1:E:400:VAL:HG21	2.01	0.41
1:F:79:GLY:O	1:F:83:VAL:HG23	2.19	0.41
1:G:105:ARG:HH22	1:G:336:GLY:H	1.68	0.41
1:H:105:ARG:HH22	1:H:338:GLN:HB2	1.83	0.41
1:I:362:MET:HA	1:I:365:MET:HE2	2.03	0.41
1:J:79:GLY:O	1:J:83:VAL:HG23	2.20	0.41
1:J:105:ARG:CZ	1:J:335:VAL:CG1	2.99	0.41
1:J:175:LYS:HG3	1:J:176:VAL:N	2.35	0.41
1:C:299:TYR:CD1	1:C:299:TYR:C	2.98	0.41
1:G:73:ILE:O	1:G:76:ALA:O	2.38	0.41
1:G:334:THR:CB	1:G:337:GLN:HB3	2.50	0.41
1:I:376:ASP:O	1:I:379:VAL:N	2.52	0.41
1:J:44:LYS:HB3	1:J:45:PRO:HD3	2.02	0.41
1:J:60:PRO:HB2	1:J:194:MET:HG3	2.02	0.41
1:J:81:VAL:HA	1:J:84:LYS:HB2	2.03	0.41
1:A:105:ARG:HH22	1:A:336:GLY:H	1.67	0.41
1:B:376:ASP:O	1:B:379:VAL:N	2.53	0.41
1:C:105:ARG:HH22	1:C:336:GLY:H	1.68	0.41
1:C:109:PRO:HB2	1:C:324:PHE:HD1	1.85	0.41
1:C:334:THR:CG2	1:C:337:GLN:CB	2.99	0.41
1:C:334:THR:CG2	1:C:337:GLN:HB3	2.50	0.41
1:C:337:GLN:HG3	1:C:340:THR:OG1	2.21	0.41
1:D:81:VAL:HA	1:D:84:LYS:HB2	2.01	0.41
1:E:334:THR:CG2	1:E:337:GLN:HB3	2.50	0.41
1:G:334:THR:O	1:G:337:GLN:N	2.48	0.41
1:I:9:GLU:OE1	1:I:10:TYR:CE2	2.74	0.41
1:J:113:ILE:N	1:J:113:ILE:HD13	2.36	0.41
1:K:79:GLY:O	1:K:83:VAL:HG23	2.20	0.41
1:L:107:PHE:HB2	1:L:234:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ARG:CZ	1:B:335:VAL:CG1	2.99	0.41
1:C:59:MET:HB2	1:C:60:PRO:HD3	2.02	0.41
1:C:60:PRO:HB2	1:C:194:MET:HG3	2.02	0.41
1:C:107:PHE:HB2	1:C:234:ALA:HB2	2.02	0.41
1:C:109:PRO:O	1:C:324:PHE:HA	2.21	0.41
1:C:119:GLY:N	1:C:120:GLN:HA	2.34	0.41
1:F:239:LEU:HB2	1:F:400:VAL:HG21	2.03	0.41
1:F:337:GLN:O	1:F:340:THR:OG1	2.38	0.41
1:G:113:ILE:HD13	1:G:113:ILE:N	2.35	0.41
1:H:44:LYS:HB3	1:H:45:PRO:HD3	2.01	0.41
1:I:44:LYS:HB3	1:I:45:PRO:HD3	2.01	0.41
1:I:105:ARG:HH21	1:I:338:GLN:NE2	2.18	0.41
1:K:334:THR:CG2	1:K:337:GLN:CB	2.98	0.41
1:A:109:PRO:HB2	1:A:324:PHE:HD1	1.86	0.41
1:A:294:ILE:HG22	1:A:295:SER:N	2.35	0.41
1:A:334:THR:CB	1:A:337:GLN:HB3	2.49	0.41
1:H:146:LEU:HB3	1:I:143:PHE:CD1	2.55	0.41
1:H:239:LEU:HB2	1:H:400:VAL:HG21	2.02	0.41
1:I:53:LEU:O	1:I:56:MET:HB3	2.20	0.41
1:J:164:ALA:HB2	1:L:197:ILE:HD13	2.03	0.41
1:L:145:ALA:HA	1:L:150:GLN:NE2	2.35	0.41
1:L:209:VAL:HA	1:L:274:VAL:HG11	2.03	0.41
1:L:275:THR:HG22	1:L:277:SER:HB3	2.01	0.41
1:G:81:VAL:HA	1:G:84:LYS:HB2	2.01	0.41
1:G:362:MET:HA	1:G:365:MET:HE2	2.02	0.41
1:L:55:LYS:O	1:L:56:MET:C	2.62	0.41
1:A:56:MET:HE3	1:B:157:PHE:HD1	1.86	0.41
1:B:53:LEU:O	1:B:56:MET:HB3	2.21	0.41
1:B:55:LYS:O	1:B:56:MET:C	2.64	0.41
1:B:105:ARG:HH22	1:B:338:GLN:HB2	1.86	0.41
1:B:205:ALA:N	1:B:206:PRO:CD	2.84	0.41
1:B:339:LEU:O	1:B:340:THR:C	2.63	0.41
1:C:121:GLN:C	1:C:371:GLY:O	2.64	0.41
1:E:144:GLY:O	1:E:145:ALA:C	2.64	0.41
1:E:215:TYR:CE1	1:E:219:GLU:HG3	2.56	0.41
1:G:195:TYR:O	1:G:198:VAL:HG12	2.21	0.41
1:G:339:LEU:O	1:G:340:THR:C	2.63	0.41
1:G:357:GLY:O	1:G:361:ILE:HD13	2.21	0.41
1:H:105:ARG:HH22	1:H:336:GLY:H	1.67	0.41
1:H:144:GLY:O	1:H:145:ALA:C	2.63	0.41
1:H:175:LYS:HG3	1:H:176:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:GLU:O	1:H:193:ALA:C	2.64	0.41
1:H:235:VAL:HG23	1:H:320:VAL:HG11	2.03	0.41
1:I:127:ALA:N	1:I:128:PRO:CD	2.84	0.41
1:I:334:THR:CG2	1:I:337:GLN:CB	2.99	0.41
1:I:334:THR:CG2	1:I:337:GLN:HB3	2.51	0.41
1:J:105:ARG:HH22	1:J:336:GLY:H	1.67	0.41
1:J:141:ASN:OD1	1:J:141:ASN:C	2.64	0.41
1:K:109:PRO:HB2	1:K:324:PHE:HD1	1.86	0.41
1:K:309:ILE:O	1:K:309:ILE:CG2	2.69	0.41
1:L:235:VAL:HG23	1:L:320:VAL:HG11	2.03	0.41
1:L:305:LEU:O	1:L:305:LEU:HG	2.20	0.41
1:L:319:GLY:O	1:L:322:THR:HG22	2.21	0.41
1:L:337:GLN:O	1:L:340:THR:OG1	2.39	0.41
1:L:391:ALA:O	1:L:395:MET:HG3	2.21	0.41
1:A:198:VAL:CG1	1:A:287:ARG:HD3	2.52	0.41
1:A:255:GLY:O	1:A:256:ILE:O	2.39	0.41
1:C:81:VAL:HA	1:C:84:LYS:HB2	2.02	0.41
1:D:80:ARG:O	1:D:82:GLY:N	2.49	0.41
1:D:376:ASP:O	1:D:379:VAL:N	2.54	0.41
1:E:334:THR:O	1:E:337:GLN:N	2.44	0.41
1:G:107:PHE:HB2	1:G:234:ALA:HB2	2.03	0.41
1:H:113:ILE:N	1:H:113:ILE:HD13	2.36	0.41
1:K:159:ILE:HD11	1:K:301:PHE:CD1	2.56	0.41
1:K:317:TYR:O	1:K:321:CYS:HB2	2.21	0.41
1:K:391:ALA:O	1:K:395:MET:HG3	2.20	0.41
1:A:145:ALA:O	1:A:149:GLY:O	2.40	0.40
1:A:376:ASP:O	1:A:379:VAL:N	2.54	0.40
1:B:44:LYS:HB3	1:B:45:PRO:HD3	2.01	0.40
1:D:197:ILE:HD12	1:E:160:ILE:CG2	2.51	0.40
1:D:205:ALA:N	1:D:206:PRO:CD	2.84	0.40
1:F:210:PHE:O	1:F:214:ALA:HB2	2.21	0.40
1:G:105:ARG:CZ	1:G:335:VAL:CG1	2.99	0.40
1:I:195:TYR:O	1:I:198:VAL:HG12	2.20	0.40
1:K:215:TYR:CE1	1:K:219:GLU:HG3	2.56	0.40
1:L:80:ARG:HD2	1:L:80:ARG:HA	1.96	0.40
1:L:127:ALA:N	1:L:128:PRO:CD	2.84	0.40
1:L:294:ILE:HG22	1:L:295:SER:N	2.35	0.40
1:A:386:ILE:HA	1:A:389:ILE:HG22	2.04	0.40
1:C:80:ARG:O	1:C:82:GLY:N	2.52	0.40
1:C:339:LEU:HD23	1:C:343:LEU:HD11	2.03	0.40
1:D:105:ARG:CZ	1:D:335:VAL:CG1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:VAL:O	1:D:117:VAL:HG23	2.21	0.40
1:D:228:LEU:HD23	1:D:228:LEU:HA	1.98	0.40
1:F:156:PHE:CD2	1:F:156:PHE:C	2.97	0.40
1:F:235:VAL:HG23	1:F:320:VAL:HG11	2.03	0.40
1:F:328:ALA:C	1:F:330:GLY:H	2.28	0.40
1:F:386:ILE:HA	1:F:389:ILE:HG22	2.04	0.40
1:G:127:ALA:N	1:G:128:PRO:CD	2.84	0.40
1:G:334:THR:CG2	1:G:337:GLN:HB3	2.50	0.40
1:G:376:ASP:O	1:G:379:VAL:N	2.55	0.40
1:J:339:LEU:O	1:J:340:THR:C	2.65	0.40
1:K:117:VAL:HG11	1:K:378:ASN:CG	2.45	0.40
1:K:127:ALA:N	1:K:128:PRO:CD	2.84	0.40
1:K:350:ILE:HG12	1:K:351:GLY:N	2.36	0.40
1:L:282:LEU:HD21	1:L:304:PRO:HA	2.02	0.40
1:A:209:VAL:HA	1:A:274:VAL:HG11	2.03	0.40
1:B:350:ILE:HG12	1:B:351:GLY:N	2.37	0.40
1:C:156:PHE:CD2	1:C:156:PHE:C	3.00	0.40
1:C:235:VAL:HG23	1:C:320:VAL:HG11	2.03	0.40
1:C:328:ALA:C	1:C:330:GLY:H	2.28	0.40
1:C:334:THR:CB	1:C:337:GLN:HB3	2.50	0.40
1:D:175:LYS:HG3	1:D:176:VAL:N	2.35	0.40
1:D:334:THR:CG2	1:D:337:GLN:HB3	2.52	0.40
1:E:60:PRO:HB2	1:E:194:MET:HG3	2.04	0.40
1:H:59:MET:HE2	1:H:146:LEU:HA	2.03	0.40
1:H:109:PRO:HB2	1:H:324:PHE:HD1	1.87	0.40
1:J:215:TYR:CE1	1:J:219:GLU:HG3	2.56	0.40
1:J:282:LEU:HD21	1:J:304:PRO:HA	2.03	0.40
1:C:117:VAL:O	1:C:117:VAL:HG23	2.22	0.40
1:C:210:PHE:O	1:C:214:ALA:HB2	2.21	0.40
1:C:357:GLY:O	1:C:361:ILE:HD13	2.22	0.40
1:D:275:THR:HG22	1:D:277:SER:HB3	2.03	0.40
1:E:213:ILE:C	1:E:213:ILE:HD12	2.46	0.40
1:G:334:THR:CG2	1:G:337:GLN:CB	2.99	0.40
1:H:198:VAL:CG1	1:H:287:ARG:HD3	2.51	0.40
1:I:145:ALA:HA	1:I:150:GLN:NE2	2.36	0.40
1:I:275:THR:HG22	1:I:277:SER:HB3	2.04	0.40
1:I:328:ALA:C	1:I:330:GLY:H	2.29	0.40
1:K:105:ARG:CZ	1:K:335:VAL:CG1	3.00	0.40
1:K:179:SER:O	1:K:180:ALA:C	2.65	0.40
1:L:105:ARG:HH22	1:L:336:GLY:H	1.68	0.40
1:L:113:ILE:HD13	1:L:113:ILE:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:195:TYR:O	1:L:198:VAL:HG12	2.22	0.40
1:L:362:MET:HA	1:L:365:MET:HE2	2.04	0.40
1:A:81:VAL:HA	1:A:84:LYS:HB2	2.03	0.40
1:D:88:TYR:CZ	1:D:92:THR:HG21	2.56	0.40
1:E:334:THR:CB	1:E:337:GLN:HB3	2.51	0.40
1:F:80:ARG:HD2	1:F:80:ARG:HA	1.95	0.40
1:I:81:VAL:HA	1:I:84:LYS:HB2	2.04	0.40
1:I:209:VAL:HA	1:I:274:VAL:HG11	2.04	0.40
1:J:294:ILE:HG22	1:J:295:SER:N	2.36	0.40
1:K:80:ARG:O	1:K:82:GLY:N	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/409 (97%)	356 (89%)	34 (8%)	8 (2%)	6	33
1	B	400/409 (98%)	355 (89%)	37 (9%)	8 (2%)	6	33
1	C	400/409 (98%)	354 (88%)	39 (10%)	7 (2%)	6	34
1	D	400/409 (98%)	354 (88%)	38 (10%)	8 (2%)	6	33
1	E	400/409 (98%)	359 (90%)	34 (8%)	7 (2%)	6	34
1	F	400/409 (98%)	356 (89%)	37 (9%)	7 (2%)	6	34
1	G	400/409 (98%)	352 (88%)	41 (10%)	7 (2%)	6	34
1	H	400/409 (98%)	352 (88%)	40 (10%)	8 (2%)	6	33
1	I	399/409 (98%)	356 (89%)	36 (9%)	7 (2%)	6	34
1	J	400/409 (98%)	359 (90%)	33 (8%)	8 (2%)	6	33
1	K	400/409 (98%)	355 (89%)	37 (9%)	8 (2%)	6	33
1	L	400/409 (98%)	355 (89%)	38 (10%)	7 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4797/4908 (98%)	4263 (89%)	444 (9%)	90 (2%)	6	34

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ILE
1	B	256	ILE
1	C	256	ILE
1	D	256	ILE
1	E	256	ILE
1	F	256	ILE
1	G	256	ILE
1	H	256	ILE
1	I	256	ILE
1	J	256	ILE
1	K	256	ILE
1	L	256	ILE
1	A	12	VAL
1	B	12	VAL
1	C	12	VAL
1	D	12	VAL
1	E	12	VAL
1	F	12	VAL
1	G	12	VAL
1	H	12	VAL
1	I	10	TYR
1	I	12	VAL
1	J	10	TYR
1	J	12	VAL
1	K	12	VAL
1	L	12	VAL
1	A	10	TYR
1	B	10	TYR
1	C	10	TYR
1	D	10	TYR
1	E	10	TYR
1	F	10	TYR
1	G	10	TYR
1	K	10	TYR
1	L	10	TYR
1	A	153	PRO
1	C	153	PRO

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Mol	Chain	Res	Type
1	E	153	PRO
1	H	10	TYR
1	K	153	PRO
1	B	153	PRO
1	D	153	PRO
1	F	153	PRO
1	G	153	PRO
1	H	153	PRO
1	H	414	LYS
1	I	153	PRO
1	J	153	PRO
1	L	153	PRO
1	A	152	LEU
1	C	152	LEU
1	D	414	LYS
1	G	152	LEU
1	J	414	LYS
1	D	152	LEU
1	E	152	LEU
1	H	152	LEU
1	J	152	LEU
1	K	152	LEU
1	F	152	LEU
1	H	118	GLY
1	I	152	LEU
1	K	118	GLY
1	L	152	LEU
1	A	118	GLY
1	B	118	GLY
1	B	152	LEU
1	C	304	PRO
1	D	118	GLY
1	E	118	GLY
1	F	110	GLY
1	F	118	GLY
1	L	110	GLY
1	B	110	GLY
1	B	304	PRO
1	C	110	GLY
1	D	110	GLY
1	E	110	GLY
1	G	110	GLY

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Mol	Chain	Res	Type
1	G	118	GLY
1	H	110	GLY
1	I	304	PRO
1	J	110	GLY
1	L	118	GLY
1	A	110	GLY
1	A	304	PRO
1	I	110	GLY
1	J	304	PRO
1	K	110	GLY
1	K	304	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	302/318 (95%)	252 (83%)	50 (17%)	2	13
1	B	303/318 (95%)	251 (83%)	52 (17%)	2	13
1	C	304/318 (96%)	255 (84%)	49 (16%)	2	14
1	D	304/318 (96%)	252 (83%)	52 (17%)	2	13
1	E	304/318 (96%)	251 (83%)	53 (17%)	2	13
1	F	304/318 (96%)	256 (84%)	48 (16%)	2	15
1	G	304/318 (96%)	254 (84%)	50 (16%)	2	14
1	H	304/318 (96%)	251 (83%)	53 (17%)	2	13
1	I	303/318 (95%)	251 (83%)	52 (17%)	2	13
1	J	304/318 (96%)	253 (83%)	51 (17%)	2	13
1	K	303/318 (95%)	254 (84%)	49 (16%)	2	14
1	L	303/318 (95%)	252 (83%)	51 (17%)	2	13
All	All	3642/3816 (95%)	3032 (83%)	610 (17%)	2	13

All (610) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	17	LEU
1	A	18	ILE
1	A	72	SER
1	A	81	VAL
1	A	98	THR
1	A	102	ILE
1	A	106	LEU
1	A	113	ILE
1	A	130	LEU
1	A	134	LEU
1	A	135	LEU
1	A	136	ASP
1	A	150	GLN
1	A	152	LEU
1	A	154	THR
1	A	155	ILE
1	A	159	ILE
1	A	160	ILE
1	A	163	ILE
1	A	197	ILE
1	A	198	VAL
1	A	219	GLU
1	A	222	VAL
1	A	225	VAL
1	A	232	THR
1	A	236	TYR
1	A	240	THR
1	A	241	LEU
1	A	250	LEU
1	A	256	ILE
1	A	270	LEU
1	A	282	LEU
1	A	299	TYR
1	A	308	THR
1	A	316	LEU
1	A	332	HIS
1	A	333	LEU
1	A	335	VAL
1	A	338	GLN
1	A	339	LEU
1	A	340	THR
1	A	341	ILE

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Mol	Chain	Res	Type
1	A	347	LEU
1	A	349	SER
1	A	350	ILE
1	A	362	MET
1	A	374	LEU
1	A	400	VAL
1	A	402	VAL
1	B	16	ILE
1	B	17	LEU
1	B	18	ILE
1	B	72	SER
1	B	81	VAL
1	B	98	THR
1	B	102	ILE
1	B	106	LEU
1	B	113	ILE
1	B	121	GLN
1	B	130	LEU
1	B	134	LEU
1	B	135	LEU
1	B	136	ASP
1	B	150	GLN
1	B	152	LEU
1	B	154	THR
1	B	155	ILE
1	B	159	ILE
1	B	160	ILE
1	B	163	ILE
1	B	197	ILE
1	B	198	VAL
1	B	219	GLU
1	B	222	VAL
1	B	225	VAL
1	B	232	THR
1	B	236	TYR
1	B	240	THR
1	B	241	LEU
1	B	250	LEU
1	B	256	ILE
1	B	270	LEU
1	B	282	LEU
1	B	299	TYR

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Mol	Chain	Res	Type
1	B	308	THR
1	B	316	LEU
1	B	322	THR
1	B	332	HIS
1	B	333	LEU
1	B	335	VAL
1	B	338	GLN
1	B	339	LEU
1	B	340	THR
1	B	341	ILE
1	B	347	LEU
1	B	349	SER
1	B	350	ILE
1	B	362	MET
1	B	374	LEU
1	B	400	VAL
1	B	402	VAL
1	C	16	ILE
1	C	17	LEU
1	C	18	ILE
1	C	72	SER
1	C	81	VAL
1	C	98	THR
1	C	102	ILE
1	C	106	LEU
1	C	113	ILE
1	C	130	LEU
1	C	135	LEU
1	C	136	ASP
1	C	150	GLN
1	C	152	LEU
1	C	154	THR
1	C	155	ILE
1	C	159	ILE
1	C	160	ILE
1	C	163	ILE
1	C	197	ILE
1	C	198	VAL
1	C	219	GLU
1	C	222	VAL
1	C	225	VAL
1	C	232	THR

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Mol	Chain	Res	Type
1	C	236	TYR
1	C	240	THR
1	C	241	LEU
1	C	250	LEU
1	C	256	ILE
1	C	270	LEU
1	C	282	LEU
1	C	299	TYR
1	C	308	THR
1	C	316	LEU
1	C	332	HIS
1	C	333	LEU
1	C	335	VAL
1	C	338	GLN
1	C	339	LEU
1	C	340	THR
1	C	341	ILE
1	C	347	LEU
1	C	349	SER
1	C	350	ILE
1	C	362	MET
1	C	374	LEU
1	C	400	VAL
1	C	402	VAL
1	D	16	ILE
1	D	17	LEU
1	D	18	ILE
1	D	72	SER
1	D	81	VAL
1	D	98	THR
1	D	102	ILE
1	D	106	LEU
1	D	113	ILE
1	D	120	GLN
1	D	130	LEU
1	D	134	LEU
1	D	135	LEU
1	D	136	ASP
1	D	150	GLN
1	D	152	LEU
1	D	154	THR
1	D	155	ILE

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Mol	Chain	Res	Type
1	D	159	ILE
1	D	160	ILE
1	D	163	ILE
1	D	179	SER
1	D	197	ILE
1	D	198	VAL
1	D	219	GLU
1	D	222	VAL
1	D	225	VAL
1	D	232	THR
1	D	236	TYR
1	D	240	THR
1	D	241	LEU
1	D	250	LEU
1	D	256	ILE
1	D	270	LEU
1	D	282	LEU
1	D	299	TYR
1	D	308	THR
1	D	316	LEU
1	D	332	HIS
1	D	333	LEU
1	D	335	VAL
1	D	338	GLN
1	D	339	LEU
1	D	340	THR
1	D	341	ILE
1	D	347	LEU
1	D	349	SER
1	D	350	ILE
1	D	362	MET
1	D	374	LEU
1	D	400	VAL
1	D	402	VAL
1	E	16	ILE
1	E	17	LEU
1	E	18	ILE
1	E	72	SER
1	E	81	VAL
1	E	98	THR
1	E	102	ILE
1	E	106	LEU

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Mol	Chain	Res	Type
1	E	113	ILE
1	E	120	GLN
1	E	121	GLN
1	E	130	LEU
1	E	134	LEU
1	E	135	LEU
1	E	136	ASP
1	E	150	GLN
1	E	152	LEU
1	E	154	THR
1	E	155	ILE
1	E	159	ILE
1	E	160	ILE
1	E	163	ILE
1	E	197	ILE
1	E	198	VAL
1	E	219	GLU
1	E	222	VAL
1	E	225	VAL
1	E	232	THR
1	E	236	TYR
1	E	240	THR
1	E	241	LEU
1	E	250	LEU
1	E	256	ILE
1	E	270	LEU
1	E	282	LEU
1	E	299	TYR
1	E	308	THR
1	E	316	LEU
1	E	322	THR
1	E	332	HIS
1	E	333	LEU
1	E	335	VAL
1	E	338	GLN
1	E	339	LEU
1	E	340	THR
1	E	341	ILE
1	E	347	LEU
1	E	349	SER
1	E	350	ILE
1	E	362	MET

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Mol	Chain	Res	Type
1	E	374	LEU
1	E	400	VAL
1	E	402	VAL
1	F	16	ILE
1	F	17	LEU
1	F	18	ILE
1	F	72	SER
1	F	81	VAL
1	F	98	THR
1	F	102	ILE
1	F	106	LEU
1	F	113	ILE
1	F	130	LEU
1	F	134	LEU
1	F	135	LEU
1	F	136	ASP
1	F	152	LEU
1	F	159	ILE
1	F	160	ILE
1	F	163	ILE
1	F	197	ILE
1	F	198	VAL
1	F	219	GLU
1	F	222	VAL
1	F	225	VAL
1	F	232	THR
1	F	236	TYR
1	F	240	THR
1	F	241	LEU
1	F	250	LEU
1	F	256	ILE
1	F	270	LEU
1	F	282	LEU
1	F	299	TYR
1	F	308	THR
1	F	316	LEU
1	F	327	ASN
1	F	332	HIS
1	F	333	LEU
1	F	335	VAL
1	F	338	GLN
1	F	339	LEU

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Mol	Chain	Res	Type
1	F	340	THR
1	F	341	ILE
1	F	347	LEU
1	F	349	SER
1	F	350	ILE
1	F	362	MET
1	F	374	LEU
1	F	400	VAL
1	F	402	VAL
1	G	16	ILE
1	G	17	LEU
1	G	18	ILE
1	G	72	SER
1	G	81	VAL
1	G	98	THR
1	G	102	ILE
1	G	106	LEU
1	G	113	ILE
1	G	120	GLN
1	G	130	LEU
1	G	135	LEU
1	G	136	ASP
1	G	150	GLN
1	G	152	LEU
1	G	154	THR
1	G	155	ILE
1	G	159	ILE
1	G	160	ILE
1	G	163	ILE
1	G	197	ILE
1	G	198	VAL
1	G	219	GLU
1	G	222	VAL
1	G	225	VAL
1	G	232	THR
1	G	236	TYR
1	G	240	THR
1	G	241	LEU
1	G	250	LEU
1	G	256	ILE
1	G	270	LEU
1	G	282	LEU

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Mol	Chain	Res	Type
1	G	299	TYR
1	G	308	THR
1	G	316	LEU
1	G	332	HIS
1	G	333	LEU
1	G	335	VAL
1	G	338	GLN
1	G	339	LEU
1	G	340	THR
1	G	341	ILE
1	G	347	LEU
1	G	349	SER
1	G	350	ILE
1	G	362	MET
1	G	374	LEU
1	G	400	VAL
1	G	402	VAL
1	H	16	ILE
1	H	17	LEU
1	H	18	ILE
1	H	72	SER
1	H	81	VAL
1	H	98	THR
1	H	102	ILE
1	H	106	LEU
1	H	113	ILE
1	H	120	GLN
1	H	121	GLN
1	H	130	LEU
1	H	134	LEU
1	H	135	LEU
1	H	136	ASP
1	H	150	GLN
1	H	152	LEU
1	H	154	THR
1	H	155	ILE
1	H	159	ILE
1	H	160	ILE
1	H	163	ILE
1	H	197	ILE
1	H	198	VAL
1	H	219	GLU

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Mol	Chain	Res	Type
1	H	222	VAL
1	H	225	VAL
1	H	232	THR
1	H	236	TYR
1	H	240	THR
1	H	241	LEU
1	H	250	LEU
1	H	256	ILE
1	H	270	LEU
1	H	282	LEU
1	H	299	TYR
1	H	308	THR
1	H	316	LEU
1	H	322	THR
1	H	332	HIS
1	H	333	LEU
1	H	335	VAL
1	H	338	GLN
1	H	339	LEU
1	H	340	THR
1	H	341	ILE
1	H	347	LEU
1	H	349	SER
1	H	350	ILE
1	H	362	MET
1	H	374	LEU
1	H	400	VAL
1	H	402	VAL
1	I	16	ILE
1	I	17	LEU
1	I	18	ILE
1	I	72	SER
1	I	81	VAL
1	I	98	THR
1	I	102	ILE
1	I	106	LEU
1	I	113	ILE
1	I	120	GLN
1	I	130	LEU
1	I	134	LEU
1	I	135	LEU
1	I	136	ASP

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Mol	Chain	Res	Type
1	I	150	GLN
1	I	152	LEU
1	I	154	THR
1	I	155	ILE
1	I	159	ILE
1	I	160	ILE
1	I	163	ILE
1	I	197	ILE
1	I	198	VAL
1	I	219	GLU
1	I	222	VAL
1	I	225	VAL
1	I	232	THR
1	I	236	TYR
1	I	240	THR
1	I	241	LEU
1	I	250	LEU
1	I	256	ILE
1	I	270	LEU
1	I	282	LEU
1	I	299	TYR
1	I	308	THR
1	I	316	LEU
1	I	322	THR
1	I	332	HIS
1	I	333	LEU
1	I	335	VAL
1	I	338	GLN
1	I	339	LEU
1	I	340	THR
1	I	341	ILE
1	I	347	LEU
1	I	349	SER
1	I	350	ILE
1	I	362	MET
1	I	374	LEU
1	I	400	VAL
1	I	402	VAL
1	J	16	ILE
1	J	17	LEU
1	J	18	ILE
1	J	72	SER

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Mol	Chain	Res	Type
1	J	81	VAL
1	J	98	THR
1	J	102	ILE
1	J	106	LEU
1	J	113	ILE
1	J	120	GLN
1	J	130	LEU
1	J	134	LEU
1	J	135	LEU
1	J	136	ASP
1	J	150	GLN
1	J	152	LEU
1	J	154	THR
1	J	155	ILE
1	J	159	ILE
1	J	160	ILE
1	J	163	ILE
1	J	197	ILE
1	J	198	VAL
1	J	219	GLU
1	J	222	VAL
1	J	225	VAL
1	J	232	THR
1	J	236	TYR
1	J	240	THR
1	J	241	LEU
1	J	250	LEU
1	J	256	ILE
1	J	270	LEU
1	J	282	LEU
1	J	299	TYR
1	J	308	THR
1	J	316	LEU
1	J	332	HIS
1	J	333	LEU
1	J	335	VAL
1	J	338	GLN
1	J	339	LEU
1	J	340	THR
1	J	341	ILE
1	J	347	LEU
1	J	349	SER

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Mol	Chain	Res	Type
1	J	350	ILE
1	J	362	MET
1	J	374	LEU
1	J	400	VAL
1	J	402	VAL
1	K	16	ILE
1	K	17	LEU
1	K	18	ILE
1	K	72	SER
1	K	81	VAL
1	K	98	THR
1	K	102	ILE
1	K	106	LEU
1	K	113	ILE
1	K	130	LEU
1	K	134	LEU
1	K	135	LEU
1	K	136	ASP
1	K	150	GLN
1	K	152	LEU
1	K	155	ILE
1	K	159	ILE
1	K	160	ILE
1	K	163	ILE
1	K	197	ILE
1	K	198	VAL
1	K	219	GLU
1	K	222	VAL
1	K	225	VAL
1	K	232	THR
1	K	236	TYR
1	K	240	THR
1	K	241	LEU
1	K	250	LEU
1	K	256	ILE
1	K	270	LEU
1	K	282	LEU
1	K	299	TYR
1	K	308	THR
1	K	316	LEU
1	K	332	HIS
1	K	333	LEU

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Mol	Chain	Res	Type
1	K	335	VAL
1	K	338	GLN
1	K	339	LEU
1	K	340	THR
1	K	341	ILE
1	K	347	LEU
1	K	349	SER
1	K	350	ILE
1	K	362	MET
1	K	374	LEU
1	K	400	VAL
1	K	402	VAL
1	L	16	ILE
1	L	17	LEU
1	L	18	ILE
1	L	72	SER
1	L	81	VAL
1	L	98	THR
1	L	102	ILE
1	L	106	LEU
1	L	113	ILE
1	L	120	GLN
1	L	130	LEU
1	L	135	LEU
1	L	136	ASP
1	L	150	GLN
1	L	152	LEU
1	L	154	THR
1	L	155	ILE
1	L	159	ILE
1	L	160	ILE
1	L	163	ILE
1	L	197	ILE
1	L	198	VAL
1	L	219	GLU
1	L	222	VAL
1	L	225	VAL
1	L	232	THR
1	L	236	TYR
1	L	240	THR
1	L	241	LEU
1	L	250	LEU

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Mol	Chain	Res	Type
1	L	256	ILE
1	L	270	LEU
1	L	282	LEU
1	L	299	TYR
1	L	308	THR
1	L	316	LEU
1	L	322	THR
1	L	332	HIS
1	L	333	LEU
1	L	335	VAL
1	L	338	GLN
1	L	339	LEU
1	L	340	THR
1	L	341	ILE
1	L	347	LEU
1	L	349	SER
1	L	350	ILE
1	L	362	MET
1	L	374	LEU
1	L	400	VAL
1	L	402	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	114	HIS
1	A	150	GLN
1	A	188	ASN
1	A	310	ASN
1	A	338	GLN
1	A	378	ASN
1	B	114	HIS
1	B	150	GLN
1	B	188	ASN
1	B	338	GLN
1	B	378	ASN
1	C	114	HIS
1	C	150	GLN
1	C	310	ASN
1	C	327	ASN
1	C	338	GLN

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Mol	Chain	Res	Type
1	D	114	HIS
1	D	150	GLN
1	D	310	ASN
1	D	338	GLN
1	D	378	ASN
1	E	114	HIS
1	E	150	GLN
1	E	188	ASN
1	E	310	ASN
1	E	338	GLN
1	E	378	ASN
1	F	114	HIS
1	F	150	GLN
1	F	310	ASN
1	F	338	GLN
1	G	114	HIS
1	G	150	GLN
1	G	310	ASN
1	G	327	ASN
1	G	338	GLN
1	H	114	HIS
1	H	150	GLN
1	H	188	ASN
1	H	310	ASN
1	H	338	GLN
1	H	378	ASN
1	I	32	HIS
1	I	114	HIS
1	I	150	GLN
1	I	188	ASN
1	I	310	ASN
1	I	338	GLN
1	I	378	ASN
1	J	114	HIS
1	J	150	GLN
1	J	188	ASN
1	J	310	ASN
1	J	318	GLN
1	J	327	ASN
1	J	338	GLN
1	J	378	ASN
1	K	37	HIS

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Mol	Chain	Res	Type
1	K	114	HIS
1	K	150	GLN
1	K	310	ASN
1	K	338	GLN
1	K	378	ASN
1	L	114	HIS
1	L	150	GLN
1	L	188	ASN
1	L	310	ASN
1	L	338	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](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	402/409 (98%)	-1.23	0 100 100	92, 145, 192, 218	0
1	B	404/409 (98%)	-1.26	0 100 100	80, 127, 179, 232	0
1	C	404/409 (98%)	-1.25	0 100 100	71, 127, 176, 212	0
1	D	404/409 (98%)	-1.27	0 100 100	98, 146, 193, 249	0
1	E	404/409 (98%)	-1.26	0 100 100	88, 138, 184, 213	0
1	F	404/409 (98%)	-1.27	0 100 100	84, 127, 179, 219	0
1	G	404/409 (98%)	-1.24	0 100 100	90, 144, 184, 218	0
1	H	404/409 (98%)	-1.21	0 100 100	87, 146, 199, 260	0
1	I	403/409 (98%)	-1.24	0 100 100	92, 143, 187, 228	0
1	J	404/409 (98%)	-1.21	0 100 100	100, 158, 199, 236	0
1	K	404/409 (98%)	-1.25	0 100 100	94, 136, 184, 240	0
1	L	404/409 (98%)	-1.27	0 100 100	88, 128, 174, 210	0
All	All	4845/4908 (98%)	-1.25	0 100 100	71, 138, 188, 260	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.