



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:57 am BST

PDB ID : 4OYE
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

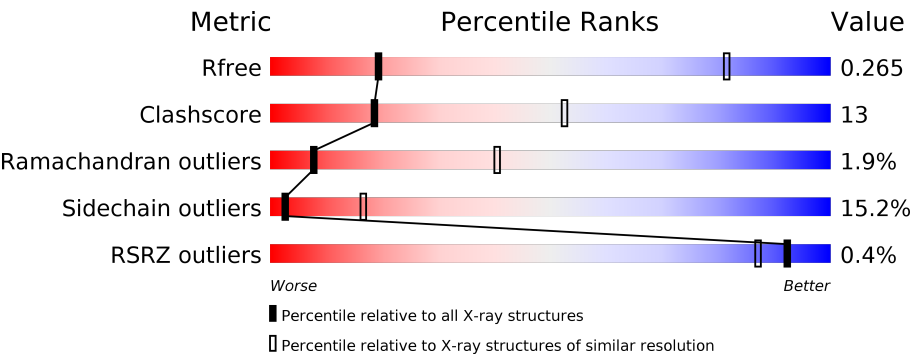
1 Overall quality at a glance i

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}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 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	<div><div></div><div>65%28%5% . .</div></div>
1	B	409	<div>%<div><div></div><div>69%24%5% .</div></div></div>
1	C	409	<div><div></div><div>66%28%. . .</div></div>
1	D	409	<div><div></div><div>68%25%5% . .</div></div>
1	E	409	<div><div></div><div>69%24%6% .</div></div>
1	F	409	<div><div></div><div>68%25%5% .</div></div>

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Mol	Chain	Length	Quality of chain
1	G	409	<div><div></div><div>68%25%5%</div><div></div></div>
1	H	409	<div><div>%</div><div></div><div>68%25%5%</div><div></div></div>
1	I	409	<div><div>%</div><div></div><div>65%28%5%</div><div></div></div>
1	J	409	<div><div>%</div><div></div><div>67%26%5%</div><div></div></div>
1	K	409	<div><div></div><div>68%24%6%</div><div></div></div>
1	L	409	<div><div></div><div>68%25%5%</div><div></div></div>

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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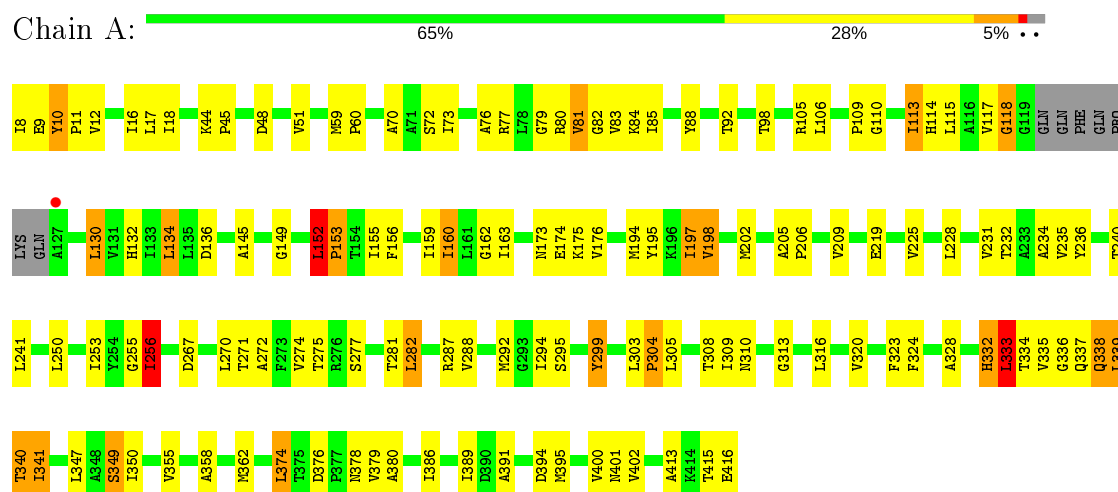
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Chain	Residue	Modelled	Actual	Comment	Reference
G	368	HIS	GLU	engineered mutation	UNP O59010
G	397	ALA	ARG	engineered mutation	UNP O59010
H	37	HIS	ASP	engineered mutation	UNP O59010
H	40	HIS	LYS	engineered mutation	UNP O59010
H	132	HIS	LYS	engineered 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

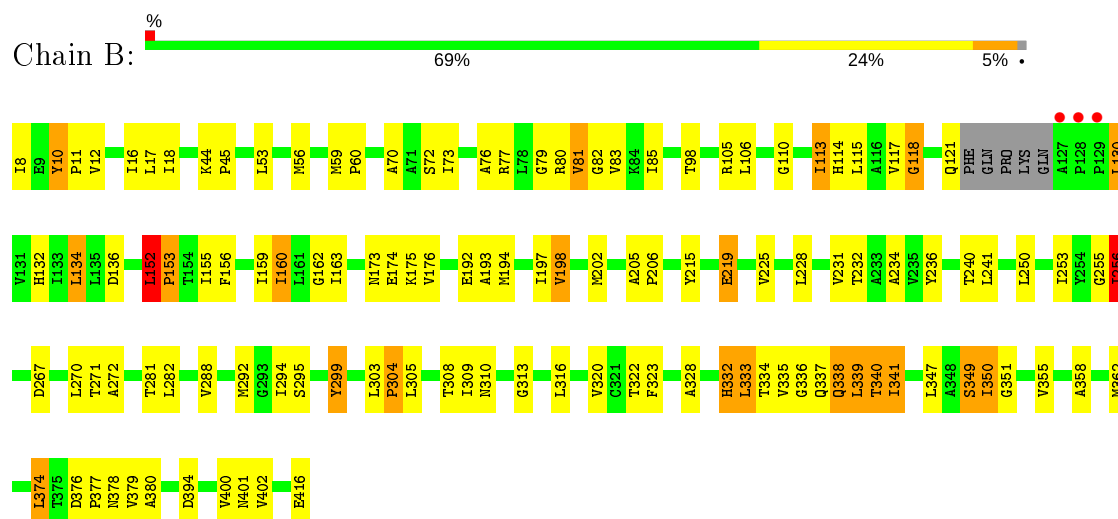
3 Residue-property plots

These plots are drawn for all protein, RNA 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: 425aa long hypothetical proton glutamate symport protein

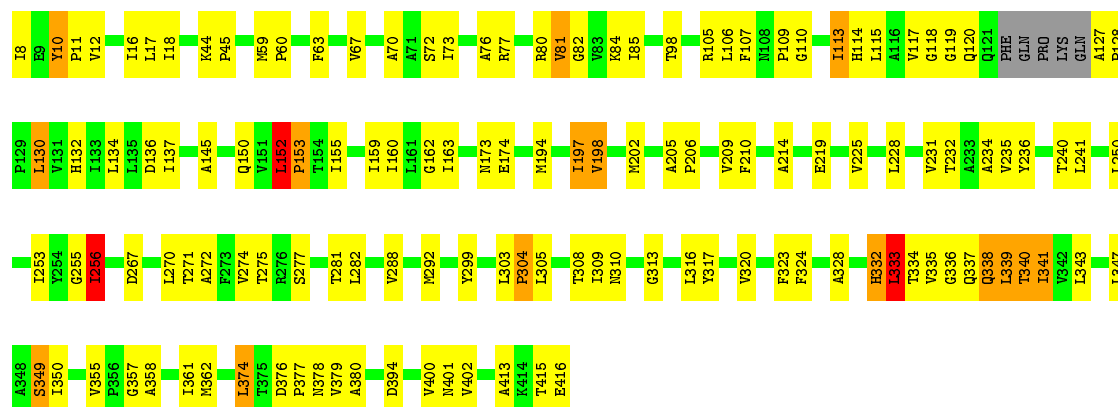


- Molecule 1: 425aa long hypothetical proton glutamate symport protein

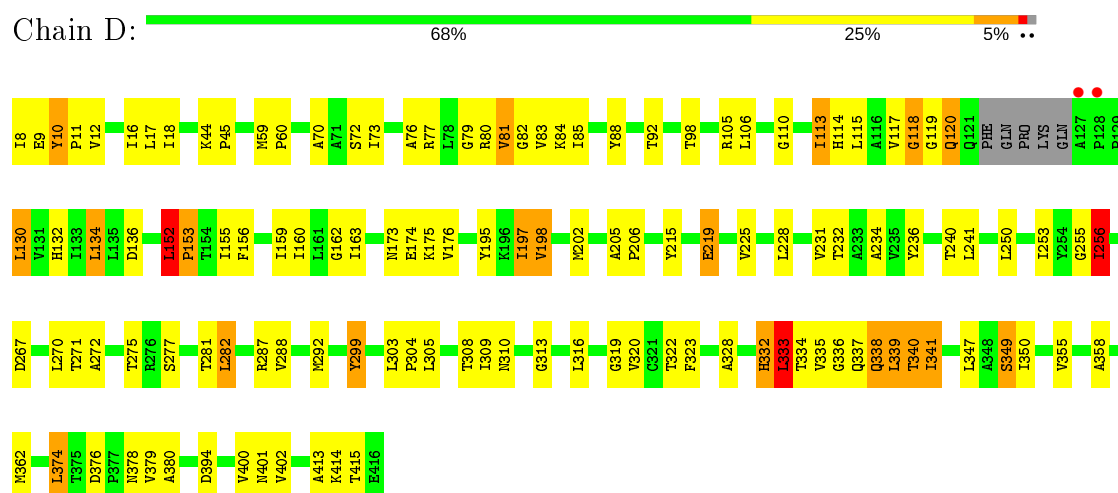


- Molecule 1: 425aa long hypothetical proton glutamate symport protein

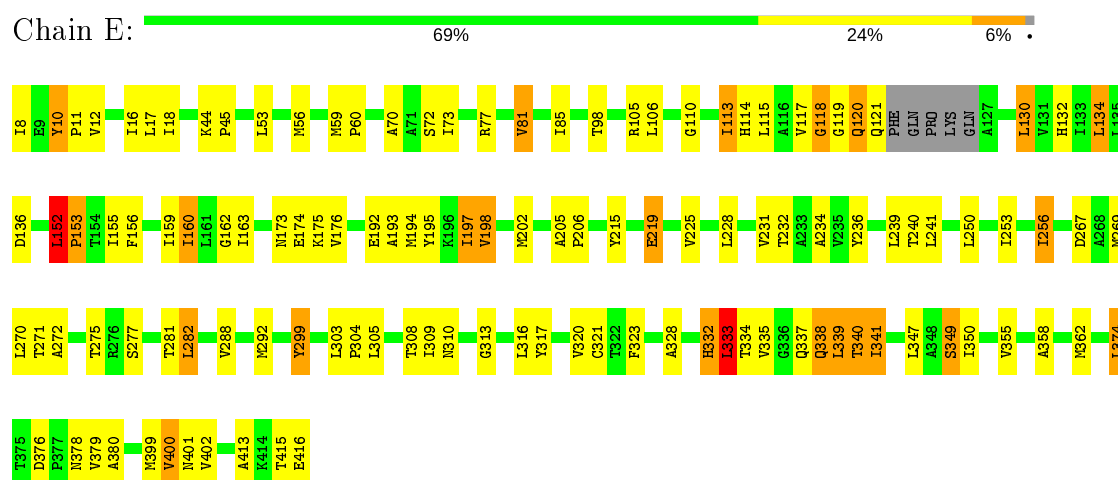




- Molecule 1: 425aa long hypothetical proton glutamate symport protein

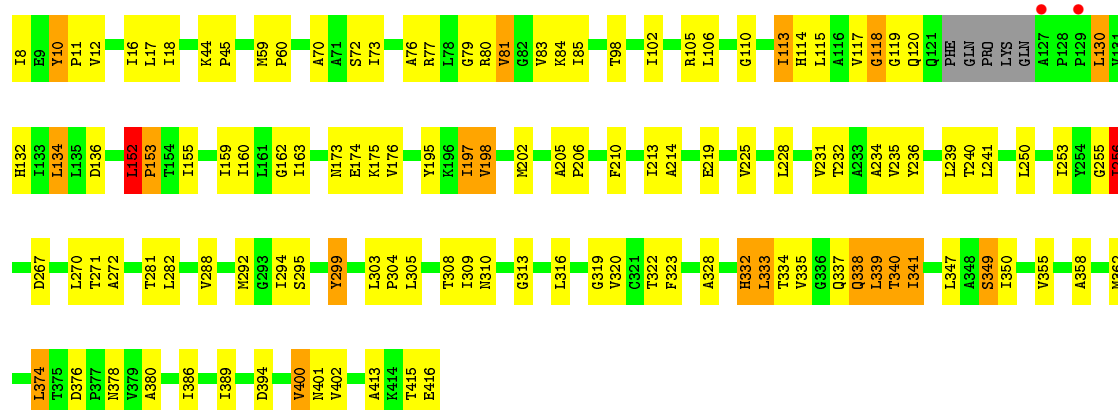


- Molecule 1: 425aa long hypothetical proton glutamate symport protein



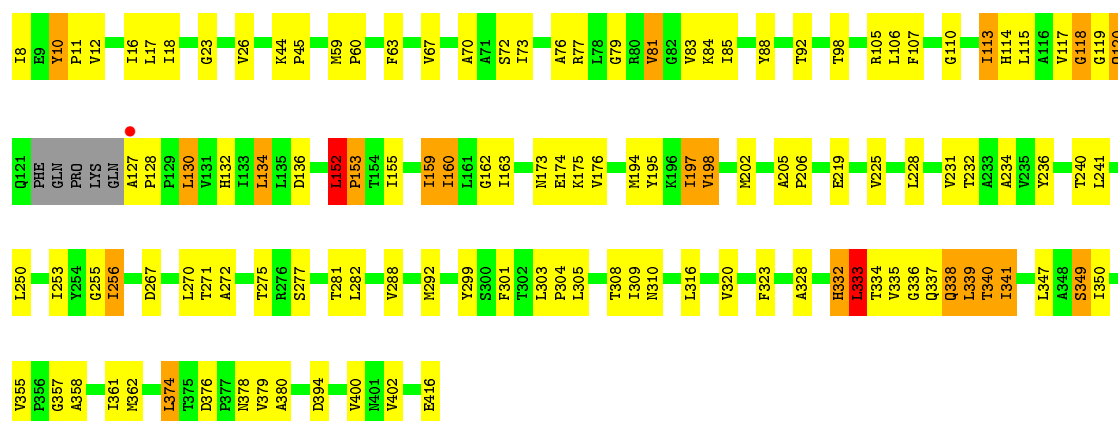
- Molecule 1: 425aa long hypothetical proton glutamate symport protein





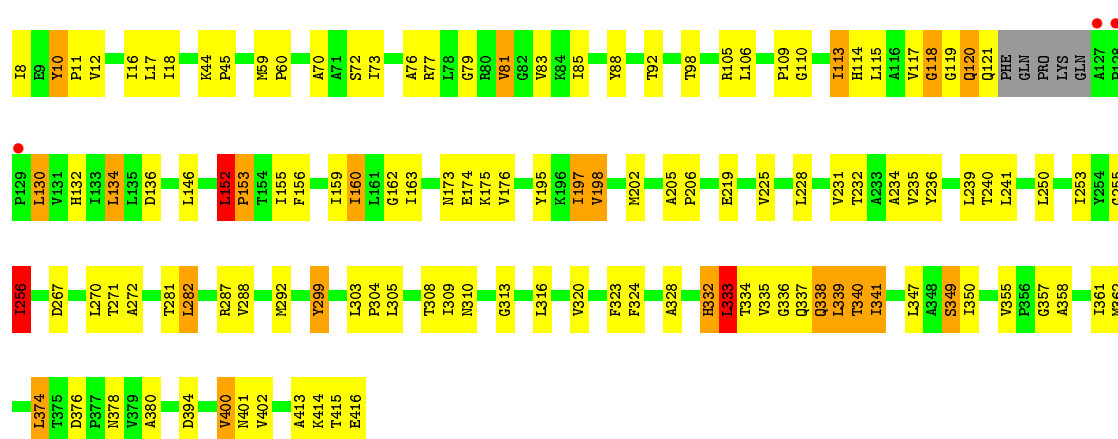
- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain G: 68% 25% 5% .



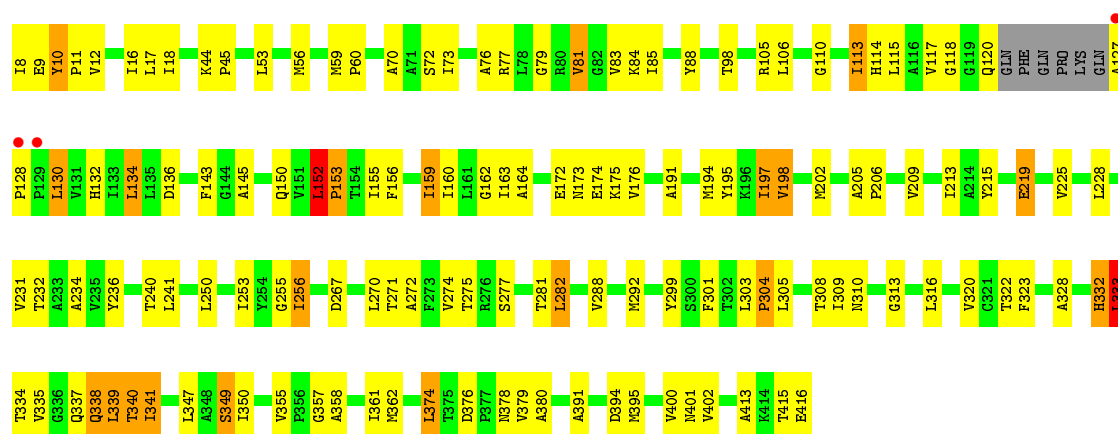
- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain H: 68% 25% 5% ..

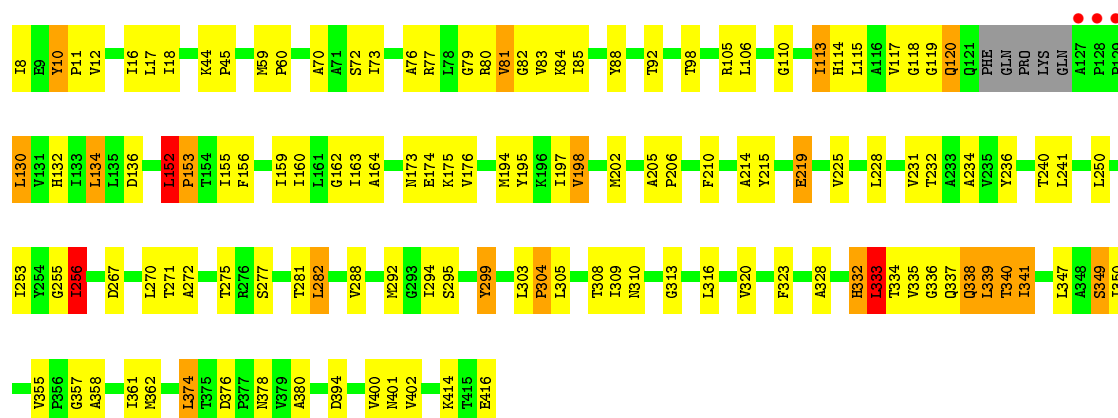


- Molecule 1: 425aa long hypothetical proton glutamate symport protein

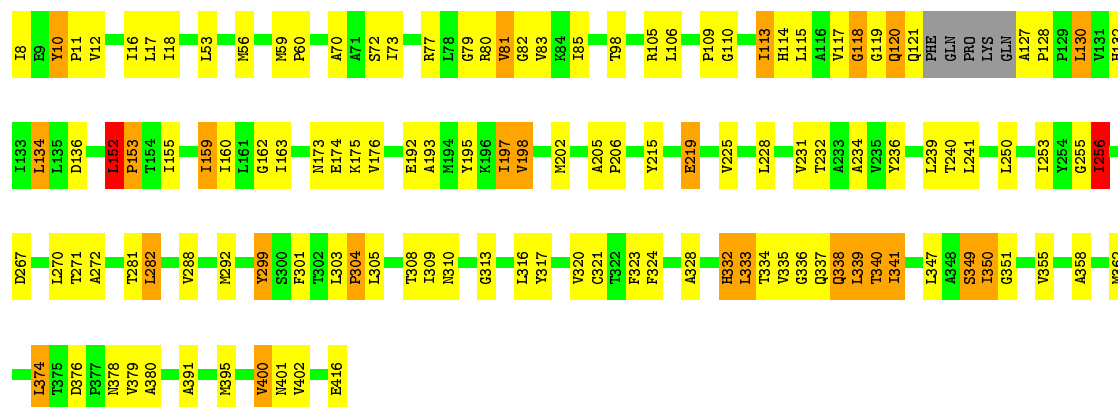
Chain I: 65% 28% 5% .



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

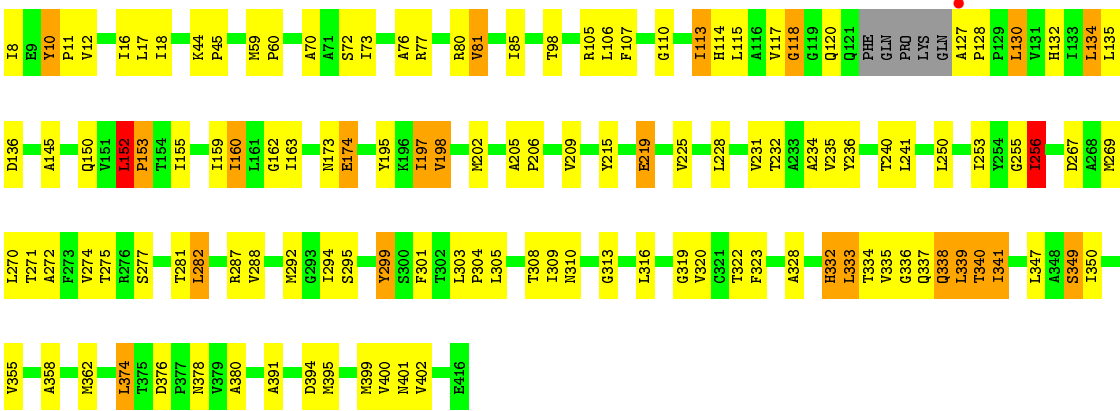


- Molecule 1: 425aa long hypothetical proton glutamate symport protein



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





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 19.98 – 4.00	Depositor EDS
% Data completeness (in resolution range)	70.3 (20.00-4.00) 70.4 (19.98-4.00)	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 (5.02%)	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)	0.21 , 61.8	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	0.87	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	0.49	0/2980	0.65	1/4074 (0.0%)
1	B	0.56	0/2994	0.69	0/4093
1	C	0.55	0/2998	0.68	1/4098 (0.0%)
1	D	0.50	0/2998	0.65	1/4098 (0.0%)
1	E	0.52	0/2998	0.67	1/4098 (0.0%)
1	F	0.56	0/2998	0.69	0/4098
1	G	0.51	0/2998	0.66	1/4098 (0.0%)
1	H	0.49	0/2998	0.67	1/4098 (0.0%)
1	I	0.52	0/2989	0.68	1/4086 (0.0%)
1	J	0.46	0/2998	0.65	1/4098 (0.0%)
1	K	0.51	0/2994	0.66	0/4094
1	L	0.55	0/2994	0.68	0/4093
All	All	0.52	0/35937	0.67	8/49126 (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	L	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	333	LEU	CA-CB-CG	5.46	127.85	115.30
1	I	333	LEU	CA-CB-CG	5.34	127.58	115.30
1	J	333	LEU	CA-CB-CG	5.27	127.43	115.30
1	C	333	LEU	CA-CB-CG	5.24	127.34	115.30
1	G	333	LEU	CA-CB-CG	5.15	127.14	115.30
1	E	333	LEU	CA-CB-CG	5.11	127.06	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	333	LEU	CA-CB-CG	5.08	126.97	115.30
1	A	333	LEU	CA-CB-CG	5.01	126.82	115.30

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	85	0
1	B	2939	0	3079	78	0
1	C	2943	0	3085	92	0
1	D	2943	0	3085	79	0
1	E	2943	0	3085	75	0
1	F	2943	0	3085	77	0
1	G	2943	0	3085	80	0
1	H	2943	0	3085	79	0
1	I	2934	0	3077	90	0
1	J	2943	0	3085	76	0
1	K	2939	0	3074	79	0
1	L	2939	0	3081	83	0
All	All	35277	0	36975	956	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 13.

All (956) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:349:SER:OG	1:B:349:SER:O	2.13	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:113:ILE:O	1:F:328:ALA:HA	1.99	0.63
1:C:73:ILE:CG1	1:I:172:GLU:CB	2.77	0.63
1:F:349:SER:O	1:F:349:SER:OG	2.13	0.63
1:A:288:VAL:O	1:A:292:MET:HB2	1.98	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:OG	1:H:349:SER:O	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:349:SER:OG	1:G:349:SER:O	2.19	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:O	1:K:349:SER:OG	2.20	0.60
1:A:334:THR:HB	1:A:337:GLN:HB3	1.84	0.60
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:113:ILE:HA	1:H:114:HIS:HB3	1.87	0.57
1:H:70:ALA:HB1	1:H:163:ILE:HD12	1.85	0.57
1:I:70:ALA:HB1	1:I:163:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:349:SER:OG	1:I:349:SER:O	2.12	0.56
1:I:77:ARG:HD3	1:I:416:GLU:CG	2.35	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:C:113:ILE:CA	1:C:114:HIS:HB3	2.35	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: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:G:334:THR:HB	1:G:337:GLN:HB3	1.86	0.56
1:D:113:ILE:HA	1:D:114:HIS:HB3	1.86	0.56
1:D:113:ILE:O	1:D:328:ALA:HA	2.05	0.56
1:H:271:THR:HG22	1:H:281:THR:HG22	1.86	0.56
1:H:77:ARG:HD3	1:H:416:GLU:CG	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:228:LEU:O	1:D:231:VAL:HG12	2.06	0.54
1:D:155:ILE:HD11	1:D:304:PRO:HB2	1.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:VAL:O	1:H:85:ILE:N	2.29	0.54
1:C:73:ILE:HG12	1:I:172:GLU:CB	2.38	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: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
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: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:G:228:LEU:O	1:G:231:VAL:HG12	2.08	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:349:SER:OG	1:J:349:SER:O	2.22	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: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:117:VAL:HG11	1:G:378:ASN:CB	2.39	0.52
1:G:73:ILE:O	1:G:77:ARG:HB2	2.09	0.52
1:I:272:ALA:HA	1:I:281:THR:HG21	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:G:332:HIS:O	1:G:333:LEU:HD13	2.09	0.51
1:E:272:ALA:HA	1:E:281:THR:HG21	1.93	0.51
1:L:288:VAL:O	1:L:292:MET:HB2	2.10	0.51
1:L:231:VAL:HG23	1:L:320:VAL:HG22	1.92	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: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: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: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:A:332:HIS:O	1:A:333:LEU:HD13	2.12	0.50
1:I:334:THR:HG22	1:I:337:GLN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:337:GLN:O	1:C:340:THR:OG1	2.28	0.50
1:H:8:ILE:O	1:H:8:ILE:HG22	2.12	0.50
1:A:349:SER:O	1:A:349:SER:OG	2.22	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: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:332:HIS:O	1:E:333:LEU:HD13	2.12	0.49
1:E:77:ARG:O	1:E:81:VAL:HG22	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:117:VAL:O	1:H:118:GLY:C	2.50	0.49
1:H:334:THR:HG22	1:H:337:GLN:HB2	1.93	0.49
1:L:272:ALA:HA	1:L:281:THR:HG21	1.94	0.49
1:L:234:ALA:HB3	1:L:320:VAL: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:I:8:ILE:HG22	1:I:8:ILE:O	2.11	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:255:GLY:O	1:I:256:ILE:O	2.31	0.49
1:I:231:VAL:HG23	1:I:320:VAL:HG22	1.95	0.49
1:L:81:VAL:O	1:L:85:ILE:N	2.30	0.49
1:L:8:ILE:O	1:L:8:ILE:HG22	2.12	0.49
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:O	1:A:8:ILE:HG22	2.13	0.49
1:B:305:LEU:O	1:B:309:ILE:HB	2.13	0.49
1:F:376:ASP:O	1:F:378:ASN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:GLN:O	1:D:340:THR:OG1	2.31	0.49
1:L:305:LEU:O	1:L:309:ILE:HB	2.12	0.49
1:F:8:ILE:O	1:F:8:ILE:HG22	2.13	0.49
1:I:255:GLY:O	1:I:256:ILE:C	2.51	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: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: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: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:I:173:ASN:OD1	1:I:174:GLU:N	2.47	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:H:255:GLY:O	1:H:256:ILE:C	2.52	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:B:117:VAL:O	1:B:118:GLY:C	2.52	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
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:E:349:SER:O	1:E:349:SER:OG	2.18	0.48
1:H:119:GLY:N	1:H:120:GLN:HA	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HG22	1:C:8:ILE:O	2.14	0.48
1:E:334:THR:HG22	1:E:337:GLN:CB	2.44	0.48
1:L:339:LEU:HD13	1:L:340:THR:H	1.78	0.48
1:A:299:TYR:CD1	1:A:299:TYR:C	2.87	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:G:117:VAL:O	1:G:118:GLY:C	2.52	0.47
1:K:73:ILE:O	1:K:77:ARG:HB2	2.14	0.47
1:B:8:ILE:O	1:B:8:ILE:HG22	2.14	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:F:173:ASN:OD1	1:F:174:GLU:N	2.48	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
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:L:130:LEU:HD12	1:L:130:LEU:C	2.35	0.47
1:E:305:LEU:O	1:E:309:ILE:HB	2.13	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: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:D:8:ILE:O	1:D:8:ILE:HG22	2.14	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: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:339:LEU:HD13	1:G:340:THR:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:ARG:O	1:G:81:VAL:HG22	2.15	0.47
1:H:332:HIS:O	1:H:333:LEU:HD13	2.14	0.47
1:I:117:VAL:HG21	1:I:378:ASN:HB2	1.97	0.47
1:I:77:ARG:O	1:I:81:VAL:HG22	2.14	0.47
1:J:117:VAL:HG21	1:J:378:ASN:HB2	1.97	0.47
1:B:339:LEU:HD13	1:B:340:THR:H	1.80	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: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:A:130:LEU:O	1:A:134:LEU:N	2.40	0.46
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:F:117:VAL:O	1:F:118:GLY:C	2.53	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:A:117:VAL:O	1:A:118:GLY:C	2.54	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: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:A:337:GLN:O	1:A:340:THR:OG1	2.34	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:117:VAL:O	1:K:118:GLY:C	2.54	0.46
1:K:332:HIS:O	1:K:333:LEU:HD22	2.14	0.46
1:L:255:GLY:O	1:L:256:ILE:C	2.53	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:130:LEU:C	1:D:130:LEU:HD12	2.36	0.46
1:I:175:LYS:HG3	1:I:176:VAL:N	2.31	0.46
1:I:73:ILE:O	1:I:76:ALA:O	2.34	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:C:334:THR:HG22	1:C:337:GLN:CB	2.46	0.46
1:E:117:VAL:O	1:E:118:GLY:C	2.55	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:L:117:VAL:O	1:L:118:GLY:C	2.53	0.46
1:D:198:VAL:CG1	1:D:287:ARG:HD3	2.46	0.45
1:I:60:PRO:HB2	1:I:194:MET:HG3	1.98	0.45
1:J:117:VAL:O	1:J:118:GLY:C	2.53	0.45
1:J:195:TYR:O	1:J:198:VAL:HG12	2.16	0.45
1:K:299:TYR:CD1	1:K:299:TYR:C	2.90	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: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: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: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:323:PHE:CE1	1:I:333:LEU:HD11	2.52	0.45
1:K:239:LEU:HB2	1:K:400:VAL:HG21	1.99	0.45
1:K:81:VAL:O	1:K:85:ILE:N	2.33	0.45
1:B:105:ARG:CZ	1:B:335:VAL:HG13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:VAL:O	1:C:118:GLY:C	2.55	0.45
1:F:77:ARG:O	1:F:81:VAL:HG22	2.15	0.45
1:G:337:GLN:O	1:G:340:THR:OG1	2.34	0.45
1:G:197:ILE:HD12	1:H:160:ILE:HG23	1.99	0.45
1:H:195:TYR:O	1:H:198:VAL:HG12	2.17	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:I:117:VAL:O	1:I:118:GLY:C	2.55	0.45
1:I:156:PHE:C	1:I:156:PHE:CD2	2.90	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
1:E:173:ASN:OD1	1:E:174:GLU:N	2.50	0.45
1:E:117:VAL:HG21	1:E:378:ASN:HB2	1.98	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:192:GLU:O	1:K:193:ALA:C	2.54	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:323:PHE:CE1	1:C:333:LEU:HD11	2.52	0.44
1:C:117:VAL:HG21	1:C:378:ASN:HB2	1.98	0.44
1:F:255:GLY:O	1:F:256:ILE:C	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:374:LEU:O	1:B:380:ALA:HB2	2.17	0.44
1:B:73:ILE:O	1:B:76:ALA:O	2.35	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:B:303:LEU:HB2	1:B:304:PRO:HD3	1.99	0.44
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:L:301:PHE:O	1:L:301:PHE:CG	2.70	0.44
1:L:105:ARG:HH21	1:L:338:GLN:NE2	2.15	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: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:D:59:MET:HB2	1:D:60:PRO:HD3	2.00	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: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:H:130:LEU:C	1:H:130:LEU:HD12	2.38	0.44
1:L:117:VAL:HG21	1:L:378:ASN:HB2	2.00	0.44
1:F:152:LEU:N	1:F:153:PRO:CD	2.81	0.44
1:G:255:GLY:O	1:G:256:ILE:C	2.55	0.44
1:J:152:LEU:N	1:J:153:PRO:CD	2.81	0.44
1:A:255:GLY:O	1:A:256:ILE:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:413:ALA:C	1:D:415:THR:H	2.21	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:H:413:ALA:C	1:H:415:THR:H	2.21	0.44
1:J:303:LEU:HB2	1:J:304:PRO:HD3	1.99	0.44
1:B:299:TYR:C	1:B:299:TYR:CD1	2.91	0.43
1:B:334:THR:O	1:B:337:GLN:N	2.43	0.43
1:B:59:MET:HB2	1:B:60:PRO:HD3	2.00	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:J:299:TYR:CD1	1:J:299:TYR:C	2.91	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
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:E:156:PHE:C	1:E:156:PHE:CD2	2.92	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:130:LEU:HD12	1:B:130:LEU:C	2.38	0.43
1:B:334:THR:CB	1:B:337:GLN:HB3	2.48	0.43
1:C:145:ALA:HA	1:C:150:GLN:NE2	2.32	0.43
1:F:197:ILE:HG12	1:F:197:ILE:H	1.71	0.43
1:F:198:VAL:O	1:F:202:MET:HG2	2.18	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:J:255:GLY:O	1:J:256:ILE:C	2.56	0.43
1:K:105:ARG:HH21	1:K:338:GLN:NE2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:130:LEU:C	1:G:130:LEU:HD12	2.38	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:F:334:THR:O	1:F:337:GLN:N	2.45	0.43
1:G:303:LEU:HB2	1:G:304:PRO:HD3	2.01	0.43
1:G:117:VAL:HG21	1:G:378:ASN:HB2	1.99	0.43
1:I:413:ALA:C	1:I:415:THR:H	2.22	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
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:N	1:I:113:ILE:HD13	2.33	0.43
1:J:105:ARG:HH21	1:J:338:GLN:NE2	2.16	0.43
1:K:255:GLY:O	1:K:256:ILE:C	2.57	0.43
1:B:334:THR:CG2	1:B:337:GLN:CB	2.96	0.43
1:D:255:GLY:O	1:D:256:ILE:C	2.57	0.43
1:D:323:PHE:CE1	1:D:333:LEU:HD11	2.53	0.43
1:E:192:GLU:O	1:E:193:ALA:C	2.57	0.43
1:H:105:ARG:CZ	1:H:335:VAL:HG13	2.49	0.43
1:H:334:THR:CG2	1:H:337:GLN:CB	2.96	0.43
1:H:117:VAL:HG21	1:H:378:ASN:HB2	2.01	0.43
1:J:156:PHE:CD2	1:J:156:PHE:C	2.92	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:C:413:ALA:C	1:C:415:THR:H	2.22	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:303:LEU:HB2	1:H:304:PRO:HD3	2.01	0.43
1:H:73:ILE:O	1:H:76:ALA:O	2.37	0.43
1:K:313:GLY:N	1:K:401:ASN:OD1	2.49	0.43
1:A:323:PHE:CE1	1:A:333:LEU:HD11	2.54	0.42
1:A:105:ARG:CZ	1:A:335:VAL:HG13	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:VAL:O	1:D:118:GLY:C	2.57	0.42
1:D:376:ASP:O	1:D:378:ASN:N	2.52	0.42
1:D:44:LYS:HB3	1:D:45:PRO:HD3	2.01	0.42
1:E:105:ARG:HH21	1:E:338:GLN:NE2	2.16	0.42
1:F:105:ARG:HH21	1:F:338:GLN:NE2	2.17	0.42
1:F:59:MET:HB2	1:F:60:PRO:HD3	2.01	0.42
1:H:339:LEU:HD13	1:H:340:THR:H	1.83	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:E:299:TYR:C	1:E:299:TYR:CD1	2.91	0.42
1:F:130:LEU:C	1:F:130:LEU:HD12	2.38	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
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:N	1:B:113:ILE:HD13	2.35	0.42
1:C:275:THR:HG22	1:C:277:SER:HB3	2.00	0.42
1:C:105:ARG:HH21	1:C:338:GLN:NE2	2.17	0.42
1:D:299:TYR:C	1:D:299:TYR:CD1	2.92	0.42
1:E:197:ILE:HG12	1:E:197:ILE:H	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:E:44:LYS:HB3	1:E:45:PRO:HD3	2.01	0.42
1:F:175:LYS:HG3	1:F:176:VAL:N	2.34	0.42
1:F:299:TYR:C	1:F:299:TYR:CD1	2.92	0.42
1:G:88:TYR:CZ	1:G:92:THR:HG21	2.54	0.42
1:H:197:ILE:HD13	1:I:164:ALA:HB2	2.01	0.42
1:J:130:LEU:C	1:J:130:LEU:HD12	2.39	0.42
1:J:59:MET:HB2	1:J:60:PRO:HD3	2.00	0.42
1:A:282:LEU:HD21	1:A:304:PRO:HA	2.01	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:9:GLU:OE1	1:A:10:TYR:CE2	2.73	0.42
1:B:81:VAL:O	1:B:85:ILE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:127:ALA:N	1:C:128:PRO:CD	2.82	0.42
1:C:80:ARG:HD2	1:C:80:ARG:HA	1.93	0.42
1:D:197:ILE:HG12	1:D:197:ILE:H	1.72	0.42
1:D:105:ARG:HH22	1:D:336:GLY:H	1.67	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
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:B:192:GLU:O	1:B:193:ALA:C	2.57	0.42
1:C:105:ARG:HH22	1:C:338:GLN:HB2	1.83	0.42
1:D:156:PHE:C	1:D:156:PHE:CD2	2.93	0.42
1:E:130:LEU:C	1:E:130:LEU:HD12	2.40	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: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:B:255:GLY:O	1:B:256:ILE:C	2.57	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:L:294:ILE:HG22	1:L:295:SER:N	2.35	0.42
1:C:105:ARG:CZ	1:C:335:VAL:CG1	2.98	0.42
1:C:130:LEU:HD12	1:C:130:LEU:C	2.40	0.42
1:D:319:GLY:O	1:D:322:THR:HG22	2.20	0.42
1:D:73:ILE:O	1:D:76:ALA:O	2.37	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:275:THR:HG22	1:J:277:SER:HB3	2.01	0.42
1:J:77:ARG:O	1:J:81:VAL:HG22	2.19	0.42
1:K:105:ARG:HH22	1:K:336:GLY:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:ARG:HH22	1:L:338:GLN:HB2	1.82	0.42
1:A:275:THR:HG22	1:A:277:SER:HB3	2.01	0.42
1:A:79:GLY:O	1:A:83:VAL:HG23	2.20	0.42
1:C:63:PHE:O	1:C:67:VAL:HG23	2.20	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:L:339:LEU:O	1:L:340:THR:C	2.58	0.42
1:B:130:LEU:O	1:B:134:LEU:N	2.42	0.41
1:B:79:GLY:O	1:B:83:VAL:HG23	2.20	0.41
1:C:137:ILE:O	1:C:153:PRO:HA	2.20	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:HG12	1:L:197:ILE:H	1.71	0.41
1:A:334:THR:O	1:A:337:GLN:N	2.47	0.41
1:B:156:PHE:C	1:B:156:PHE:CD2	2.93	0.41
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: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:J:175:LYS:HG3	1:J:176:VAL:N	2.35	0.41
1:J:105:ARG:CZ	1:J:335:VAL:CG1	2.99	0.41
1:J:79:GLY:O	1:J:83:VAL:HG23	2.20	0.41
1:G:334:THR:CB	1:G:337:GLN:HB3	2.50	0.41
1:G:73:ILE:O	1:G:76:ALA:O	2.38	0.41
1:I:376:ASP:O	1:I:379:VAL:N	2.52	0.41
1:J:60:PRO:HB2	1:J:194:MET:HG3	2.02	0.41
1:J:44:LYS:HB3	1:J:45:PRO:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:299:TYR:CD1	1:H:299:TYR:C	2.94	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
1:B:105:ARG:CZ	1:B:335:VAL:CG1	2.99	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:C:60:PRO:HB2	1:C:194:MET:HG3	2.02	0.41
1:C:59:MET:HB2	1:C:60:PRO:HD3	2.02	0.41
1:F:337:GLN:O	1:F:340:THR:OG1	2.38	0.41
1:F:239:LEU:HB2	1:F:400:VAL:HG21	2.03	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:105:ARG:HH21	1:I:338:GLN:NE2	2.18	0.41
1:I:44:LYS:HB3	1:I:45:PRO:HD3	2.01	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:L:145:ALA:HA	1:L:150:GLN:NE2	2.35	0.41
1:J:164:ALA:HB2	1:L:197:ILE:HD13	2.03	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:A:156:PHE:CD2	1:A:156:PHE:C	2.93	0.41
1:G:81:VAL:HA	1:G:84:LYS:HB2	2.01	0.41
1:A:413:ALA:C	1:A:415:THR:H	2.24	0.41
1:G:195:TYR:O	1:G:198:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:ARG:HH22	1:H:336:GLY:H	1.67	0.41
1:H:175:LYS:HG3	1:H:176:VAL:N	2.36	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:K:109:PRO:HB2	1:K:324:PHE:HD1	1.86	0.41
1:L:235:VAL:HG23	1:L:320:VAL:HG11	2.03	0.41
1:L:319:GLY:O	1:L:322:THR:HG22	2.21	0.41
1:L:391:ALA:O	1:L:395:MET:HG3	2.21	0.41
1:B:205:ALA:N	1:B:206:PRO:CD	2.84	0.41
1:B:105:ARG:HH22	1:B:338:GLN:HB2	1.86	0.41
1:B:53:LEU:O	1:B:56:MET:HB3	2.21	0.41
1:E:215:TYR:CE1	1:E:219:GLU:HG3	2.56	0.41
1:E:413:ALA:C	1:E:415:THR:H	2.24	0.41
1:G:357:GLY:O	1:G:361:ILE:HD13	2.21	0.41
1:H:156:PHE:C	1:H:156:PHE:CD2	2.93	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:K:309:ILE:O	1:K:309:ILE:CG2	2.69	0.41
1:L:305:LEU:HG	1:L:305:LEU:O	2.20	0.41
1:L:337:GLN:O	1:L:340:THR:OG1	2.39	0.41
1:A:255:GLY:O	1:A:256:ILE:O	2.39	0.41
1:A:198:VAL:CG1	1:A:287:ARG:HD3	2.52	0.41
1:C:81:VAL:HA	1:C:84:LYS:HB2	2.02	0.41
1:D:376:ASP:O	1:D:379:VAL:N	2.54	0.41
1:D:80:ARG:O	1:D:82:GLY:N	2.49	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:HD13	1:H:113:ILE:N	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:C:255:GLY:O	1:C:256:ILE:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:213:ILE:C	1:I:213:ILE:HD12	2.41	0.40
1:K:215:TYR:CE1	1:K:219:GLU:HG3	2.56	0.40
1:L:127:ALA:N	1:L:128:PRO:CD	2.84	0.40
1:L:80:ARG:HD2	1:L:80:ARG:HA	1.96	0.40
1:A:386:ILE:HA	1:A:389:ILE:HG22	2.04	0.40
1:C:339:LEU:HD23	1:C:343:LEU:HD11	2.03	0.40
1:C:80:ARG:O	1:C:82:GLY:N	2.52	0.40
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:D:105:ARG:CZ	1:D:335:VAL:CG1	2.99	0.40
1:F:213:ILE:HD12	1:F:213:ILE:C	2.42	0.40
1:F:235:VAL:HG23	1:F:320:VAL:HG11	2.03	0.40
1:F:386:ILE:HA	1:F:389:ILE:HG22	2.04	0.40
1:F:413:ALA:C	1:F:415:THR:H	2.25	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:K:127:ALA:N	1:K:128:PRO:CD	2.84	0.40
1:K:130:LEU:C	1:K:130:LEU:HD12	2.41	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:235:VAL:HG23	1:C:320:VAL:HG11	2.03	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: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:L:299:TYR:C	1:L:299:TYR:CD1	2.94	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: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:K:105:ARG:CZ	1:K:335:VAL:CG1	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:113:ILE:N	1:L:113:ILE:HD13	2.37	0.40
1:L:195:TYR:O	1:L:198:VAL:HG12	2.22	0.40
1:L:105:ARG:HH22	1:L:336:GLY:H	1.68	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:209:VAL:HA	1:I:274:VAL:HG11	2.04	0.40
1:I:81:VAL:HA	1:I:84:LYS:HB2	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%)	7	40
1	B	400/409 (98%)	355 (89%)	37 (9%)	8 (2%)	7	40
1	C	400/409 (98%)	354 (88%)	39 (10%)	7 (2%)	8	41
1	D	400/409 (98%)	354 (88%)	38 (10%)	8 (2%)	7	40
1	E	400/409 (98%)	359 (90%)	34 (8%)	7 (2%)	8	41
1	F	400/409 (98%)	356 (89%)	37 (9%)	7 (2%)	8	41
1	G	400/409 (98%)	352 (88%)	41 (10%)	7 (2%)	8	41
1	H	400/409 (98%)	352 (88%)	40 (10%)	8 (2%)	7	40
1	I	399/409 (98%)	356 (89%)	36 (9%)	7 (2%)	8	41
1	J	400/409 (98%)	359 (90%)	33 (8%)	8 (2%)	7	40
1	K	400/409 (98%)	355 (89%)	37 (9%)	8 (2%)	7	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	400/409 (98%)	355 (89%)	38 (10%)	7 (2%)	8	41
All	All	4797/4908 (98%)	4263 (89%)	444 (9%)	90 (2%)	8	40

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

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Mol	Chain	Res	Type
1	C	153	PRO
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

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Mol	Chain	Res	Type
1	G	110	GLY
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%)	257 (85%)	45 (15%)	3	17
1	B	303/318 (95%)	256 (84%)	47 (16%)	2	16
1	C	304/318 (96%)	258 (85%)	46 (15%)	3	17
1	D	304/318 (96%)	258 (85%)	46 (15%)	3	17
1	E	304/318 (96%)	258 (85%)	46 (15%)	3	17
1	F	304/318 (96%)	259 (85%)	45 (15%)	3	17
1	G	304/318 (96%)	259 (85%)	45 (15%)	3	17
1	H	304/318 (96%)	257 (84%)	47 (16%)	2	16
1	I	303/318 (95%)	257 (85%)	46 (15%)	3	16
1	J	304/318 (96%)	258 (85%)	46 (15%)	3	17
1	K	303/318 (95%)	257 (85%)	46 (15%)	3	16
1	L	303/318 (95%)	256 (84%)	47 (16%)	2	16
All	All	3642/3816 (95%)	3090 (85%)	552 (15%)	3	16

All (552) 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	106	LEU
1	A	113	ILE
1	A	130	LEU
1	A	132	HIS
1	A	134	LEU
1	A	136	ASP
1	A	152	LEU
1	A	159	ILE
1	A	160	ILE
1	A	197	ILE
1	A	198	VAL
1	A	219	GLU
1	A	225	VAL
1	A	232	THR
1	A	236	TYR
1	A	240	THR
1	A	241	LEU
1	A	256	ILE
1	A	267	ASP
1	A	270	LEU
1	A	282	LEU
1	A	299	TYR
1	A	308	THR
1	A	310	ASN
1	A	316	LEU
1	A	332	HIS
1	A	333	LEU
1	A	338	GLN
1	A	339	LEU
1	A	340	THR
1	A	341	ILE
1	A	347	LEU
1	A	349	SER
1	A	350	ILE
1	A	362	MET
1	A	374	LEU
1	A	394	ASP

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Mol	Chain	Res	Type
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	106	LEU
1	B	113	ILE
1	B	121	GLN
1	B	130	LEU
1	B	132	HIS
1	B	134	LEU
1	B	136	ASP
1	B	152	LEU
1	B	159	ILE
1	B	160	ILE
1	B	197	ILE
1	B	198	VAL
1	B	219	GLU
1	B	225	VAL
1	B	232	THR
1	B	236	TYR
1	B	240	THR
1	B	241	LEU
1	B	256	ILE
1	B	267	ASP
1	B	270	LEU
1	B	282	LEU
1	B	299	TYR
1	B	308	THR
1	B	310	ASN
1	B	316	LEU
1	B	322	THR
1	B	332	HIS
1	B	333	LEU
1	B	338	GLN
1	B	339	LEU
1	B	340	THR
1	B	341	ILE
1	B	347	LEU

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Mol	Chain	Res	Type
1	B	349	SER
1	B	350	ILE
1	B	362	MET
1	B	374	LEU
1	B	394	ASP
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	106	LEU
1	C	113	ILE
1	C	130	LEU
1	C	132	HIS
1	C	134	LEU
1	C	136	ASP
1	C	152	LEU
1	C	159	ILE
1	C	160	ILE
1	C	197	ILE
1	C	198	VAL
1	C	219	GLU
1	C	225	VAL
1	C	232	THR
1	C	236	TYR
1	C	240	THR
1	C	241	LEU
1	C	256	ILE
1	C	267	ASP
1	C	270	LEU
1	C	282	LEU
1	C	299	TYR
1	C	308	THR
1	C	310	ASN
1	C	316	LEU
1	C	317	TYR
1	C	332	HIS
1	C	333	LEU
1	C	338	GLN

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Mol	Chain	Res	Type
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	394	ASP
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	106	LEU
1	D	113	ILE
1	D	120	GLN
1	D	130	LEU
1	D	132	HIS
1	D	134	LEU
1	D	136	ASP
1	D	152	LEU
1	D	159	ILE
1	D	160	ILE
1	D	197	ILE
1	D	198	VAL
1	D	219	GLU
1	D	225	VAL
1	D	232	THR
1	D	236	TYR
1	D	240	THR
1	D	241	LEU
1	D	256	ILE
1	D	267	ASP
1	D	270	LEU
1	D	282	LEU
1	D	299	TYR
1	D	308	THR
1	D	310	ASN

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Mol	Chain	Res	Type
1	D	316	LEU
1	D	332	HIS
1	D	333	LEU
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	394	ASP
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	106	LEU
1	E	113	ILE
1	E	120	GLN
1	E	121	GLN
1	E	130	LEU
1	E	132	HIS
1	E	134	LEU
1	E	136	ASP
1	E	152	LEU
1	E	159	ILE
1	E	160	ILE
1	E	197	ILE
1	E	198	VAL
1	E	219	GLU
1	E	225	VAL
1	E	232	THR
1	E	236	TYR
1	E	240	THR
1	E	241	LEU
1	E	256	ILE
1	E	267	ASP

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Mol	Chain	Res	Type
1	E	270	LEU
1	E	282	LEU
1	E	299	TYR
1	E	308	THR
1	E	310	ASN
1	E	316	LEU
1	E	332	HIS
1	E	333	LEU
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
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	106	LEU
1	F	113	ILE
1	F	130	LEU
1	F	132	HIS
1	F	134	LEU
1	F	136	ASP
1	F	152	LEU
1	F	159	ILE
1	F	160	ILE
1	F	197	ILE
1	F	198	VAL
1	F	219	GLU
1	F	225	VAL
1	F	232	THR
1	F	236	TYR
1	F	240	THR
1	F	241	LEU

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Mol	Chain	Res	Type
1	F	256	ILE
1	F	267	ASP
1	F	270	LEU
1	F	282	LEU
1	F	299	TYR
1	F	308	THR
1	F	310	ASN
1	F	316	LEU
1	F	332	HIS
1	F	333	LEU
1	F	338	GLN
1	F	339	LEU
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	394	ASP
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	106	LEU
1	G	113	ILE
1	G	120	GLN
1	G	130	LEU
1	G	132	HIS
1	G	134	LEU
1	G	136	ASP
1	G	152	LEU
1	G	159	ILE
1	G	160	ILE
1	G	197	ILE
1	G	198	VAL
1	G	219	GLU
1	G	225	VAL

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Mol	Chain	Res	Type
1	G	232	THR
1	G	236	TYR
1	G	240	THR
1	G	241	LEU
1	G	267	ASP
1	G	270	LEU
1	G	282	LEU
1	G	299	TYR
1	G	308	THR
1	G	310	ASN
1	G	316	LEU
1	G	332	HIS
1	G	333	LEU
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	394	ASP
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	106	LEU
1	H	113	ILE
1	H	120	GLN
1	H	121	GLN
1	H	130	LEU
1	H	132	HIS
1	H	134	LEU
1	H	136	ASP
1	H	152	LEU
1	H	159	ILE
1	H	160	ILE

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Mol	Chain	Res	Type
1	H	197	ILE
1	H	198	VAL
1	H	219	GLU
1	H	225	VAL
1	H	232	THR
1	H	236	TYR
1	H	240	THR
1	H	241	LEU
1	H	256	ILE
1	H	267	ASP
1	H	270	LEU
1	H	282	LEU
1	H	299	TYR
1	H	308	THR
1	H	310	ASN
1	H	316	LEU
1	H	332	HIS
1	H	333	LEU
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	394	ASP
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	106	LEU
1	I	113	ILE
1	I	120	GLN
1	I	130	LEU
1	I	132	HIS
1	I	134	LEU

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Mol	Chain	Res	Type
1	I	136	ASP
1	I	152	LEU
1	I	159	ILE
1	I	160	ILE
1	I	197	ILE
1	I	198	VAL
1	I	219	GLU
1	I	225	VAL
1	I	232	THR
1	I	236	TYR
1	I	240	THR
1	I	241	LEU
1	I	267	ASP
1	I	270	LEU
1	I	282	LEU
1	I	299	TYR
1	I	308	THR
1	I	310	ASN
1	I	316	LEU
1	I	322	THR
1	I	332	HIS
1	I	333	LEU
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	394	ASP
1	I	400	VAL
1	I	402	VAL
1	J	16	ILE
1	J	17	LEU
1	J	18	ILE
1	J	72	SER
1	J	81	VAL
1	J	98	THR
1	J	106	LEU
1	J	113	ILE

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Mol	Chain	Res	Type
1	J	120	GLN
1	J	130	LEU
1	J	132	HIS
1	J	134	LEU
1	J	136	ASP
1	J	152	LEU
1	J	159	ILE
1	J	160	ILE
1	J	197	ILE
1	J	198	VAL
1	J	219	GLU
1	J	225	VAL
1	J	232	THR
1	J	236	TYR
1	J	240	THR
1	J	241	LEU
1	J	256	ILE
1	J	267	ASP
1	J	270	LEU
1	J	282	LEU
1	J	299	TYR
1	J	308	THR
1	J	310	ASN
1	J	316	LEU
1	J	332	HIS
1	J	333	LEU
1	J	338	GLN
1	J	339	LEU
1	J	340	THR
1	J	341	ILE
1	J	347	LEU
1	J	349	SER
1	J	350	ILE
1	J	362	MET
1	J	374	LEU
1	J	394	ASP
1	J	400	VAL
1	J	402	VAL
1	K	16	ILE
1	K	17	LEU
1	K	18	ILE
1	K	72	SER

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Mol	Chain	Res	Type
1	K	81	VAL
1	K	98	THR
1	K	106	LEU
1	K	113	ILE
1	K	120	GLN
1	K	121	GLN
1	K	130	LEU
1	K	132	HIS
1	K	134	LEU
1	K	136	ASP
1	K	152	LEU
1	K	159	ILE
1	K	160	ILE
1	K	197	ILE
1	K	198	VAL
1	K	219	GLU
1	K	225	VAL
1	K	232	THR
1	K	236	TYR
1	K	240	THR
1	K	241	LEU
1	K	256	ILE
1	K	267	ASP
1	K	270	LEU
1	K	282	LEU
1	K	299	TYR
1	K	308	THR
1	K	310	ASN
1	K	316	LEU
1	K	332	HIS
1	K	333	LEU
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

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Mol	Chain	Res	Type
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	106	LEU
1	L	113	ILE
1	L	120	GLN
1	L	130	LEU
1	L	132	HIS
1	L	134	LEU
1	L	135	LEU
1	L	136	ASP
1	L	152	LEU
1	L	159	ILE
1	L	160	ILE
1	L	197	ILE
1	L	198	VAL
1	L	219	GLU
1	L	225	VAL
1	L	232	THR
1	L	236	TYR
1	L	240	THR
1	L	241	LEU
1	L	256	ILE
1	L	267	ASP
1	L	270	LEU
1	L	282	LEU
1	L	299	TYR
1	L	308	THR
1	L	310	ASN
1	L	316	LEU
1	L	332	HIS
1	L	333	LEU
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

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Mol	Chain	Res	Type
1	L	362	MET
1	L	374	LEU
1	L	394	ASP
1	L	400	VAL
1	L	402	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	337	GLN
1	A	338	GLN
1	B	150	GLN
1	B	337	GLN
1	B	338	GLN
1	C	150	GLN
1	C	337	GLN
1	C	338	GLN
1	D	150	GLN
1	D	310	ASN
1	D	337	GLN
1	D	338	GLN
1	E	150	GLN
1	E	337	GLN
1	E	338	GLN
1	F	150	GLN
1	F	337	GLN
1	F	338	GLN
1	G	150	GLN
1	G	337	GLN
1	G	338	GLN
1	H	150	GLN
1	H	310	ASN
1	H	337	GLN
1	H	338	GLN
1	I	150	GLN
1	I	337	GLN
1	I	338	GLN
1	J	150	GLN
1	J	310	ASN
1	J	337	GLN
1	J	338	GLN

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Mol	Chain	Res	Type
1	K	150	GLN
1	K	337	GLN
1	K	338	GLN
1	L	150	GLN
1	L	337	GLN
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 carbohydrates 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 ⓘ

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	402/409 (98%)	-0.66	1 (0%) 95 93	92, 145, 192, 218	0
1	B	404/409 (98%)	-0.65	3 (0%) 87 82	80, 127, 179, 232	0
1	C	404/409 (98%)	-0.66	0 100 100	71, 127, 176, 212	0
1	D	404/409 (98%)	-0.65	2 (0%) 91 85	98, 146, 193, 249	0
1	E	404/409 (98%)	-0.66	0 100 100	88, 138, 184, 213	0
1	F	404/409 (98%)	-0.68	2 (0%) 91 85	84, 127, 179, 219	0
1	G	404/409 (98%)	-0.66	1 (0%) 95 93	90, 144, 184, 218	0
1	H	404/409 (98%)	-0.65	3 (0%) 87 82	87, 146, 199, 260	0
1	I	403/409 (98%)	-0.62	3 (0%) 87 82	92, 143, 187, 228	0
1	J	404/409 (98%)	-0.67	3 (0%) 87 82	100, 158, 199, 236	0
1	K	404/409 (98%)	-0.67	0 100 100	94, 137, 184, 240	0
1	L	404/409 (98%)	-0.72	1 (0%) 95 93	88, 128, 174, 210	0
All	All	4845/4908 (98%)	-0.66	19 (0%) 92 87	71, 138, 188, 260	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	127	ALA	6.8
1	A	127	ALA	5.6
1	B	127	ALA	5.3
1	I	127	ALA	5.0
1	H	127	ALA	4.8
1	D	128	PRO	4.5
1	J	128	PRO	4.4
1	I	128	PRO	4.1
1	J	129	PRO	4.1
1	H	128	PRO	3.6
1	F	127	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	128	PRO	3.4
1	F	129	PRO	3.3
1	J	127	ALA	2.7
1	G	127	ALA	2.5
1	I	129	PRO	2.5
1	H	129	PRO	2.4
1	L	127	ALA	2.4
1	B	129	PRO	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.