



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 04:28 AM EDT

PDB ID : 4QFK
Title : Crystal structure of dipeptide binding protein from pseudoalteromonas sp. SM9913
Authors : Li, C.Y.; Zhang, Y.Z.
Deposited on : 2014-05-21
Resolution : 2.29 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

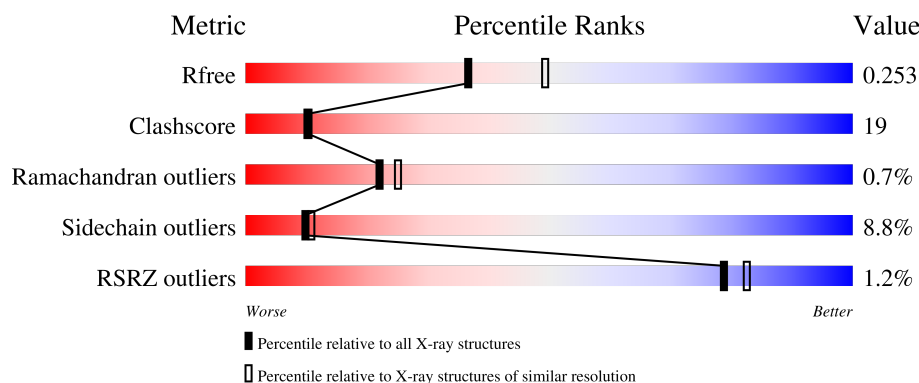
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	541	<div> <div>2%</div> <div>61% 29% 7%</div> </div>
1	B	541	<div> <div>2%</div> <div>63% 26% 5% 7%</div> </div>
1	C	541	<div> <div>2%</div> <div>60% 28% 5% 7%</div> </div>
1	D	541	<div> <div>2%</div> <div>64% 24% 5% 7%</div> </div>
1	E	541	<div> <div>2%</div> <div>59% 30% 7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	541	<div><div><div>%</div><div><div></div><div>60%</div><div>27%</div><div>6%</div><div>7%</div></div></div></div>
1	G	541	<div><div><div>2%</div><div><div></div><div>62%</div><div>26%</div><div>5%</div><div>7%</div></div></div></div>
1	H	541	<div><div><div></div><div><div></div><div>64%</div><div>24%</div><div>5%</div><div>7%</div></div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34170 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 ABC transporter periplasmic peptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	A	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	B	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	C	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	D	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	E	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	F	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			
1	G	505	Total	C	N	O	S	0	0	0
			4061	2605	685	757	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	536	HIS	-	expression tag	UNP A7Y7W1
H	537	HIS	-	expression tag	UNP A7Y7W1
H	538	HIS	-	expression tag	UNP A7Y7W1
H	539	HIS	-	expression tag	UNP A7Y7W1
H	540	HIS	-	expression tag	UNP A7Y7W1
H	541	HIS	-	expression tag	UNP A7Y7W1
A	536	HIS	-	expression tag	UNP A7Y7W1
A	537	HIS	-	expression tag	UNP A7Y7W1
A	538	HIS	-	expression tag	UNP A7Y7W1
A	539	HIS	-	expression tag	UNP A7Y7W1
A	540	HIS	-	expression tag	UNP A7Y7W1
A	541	HIS	-	expression tag	UNP A7Y7W1
B	536	HIS	-	expression tag	UNP A7Y7W1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	537	HIS	-	expression tag	UNP A7Y7W1
B	538	HIS	-	expression tag	UNP A7Y7W1
B	539	HIS	-	expression tag	UNP A7Y7W1
B	540	HIS	-	expression tag	UNP A7Y7W1
B	541	HIS	-	expression tag	UNP A7Y7W1
C	536	HIS	-	expression tag	UNP A7Y7W1
C	537	HIS	-	expression tag	UNP A7Y7W1
C	538	HIS	-	expression tag	UNP A7Y7W1
C	539	HIS	-	expression tag	UNP A7Y7W1
C	540	HIS	-	expression tag	UNP A7Y7W1
C	541	HIS	-	expression tag	UNP A7Y7W1
D	536	HIS	-	expression tag	UNP A7Y7W1
D	537	HIS	-	expression tag	UNP A7Y7W1
D	538	HIS	-	expression tag	UNP A7Y7W1
D	539	HIS	-	expression tag	UNP A7Y7W1
D	540	HIS	-	expression tag	UNP A7Y7W1
D	541	HIS	-	expression tag	UNP A7Y7W1
E	536	HIS	-	expression tag	UNP A7Y7W1
E	537	HIS	-	expression tag	UNP A7Y7W1
E	538	HIS	-	expression tag	UNP A7Y7W1
E	539	HIS	-	expression tag	UNP A7Y7W1
E	540	HIS	-	expression tag	UNP A7Y7W1
E	541	HIS	-	expression tag	UNP A7Y7W1
F	536	HIS	-	expression tag	UNP A7Y7W1
F	537	HIS	-	expression tag	UNP A7Y7W1
F	538	HIS	-	expression tag	UNP A7Y7W1
F	539	HIS	-	expression tag	UNP A7Y7W1
F	540	HIS	-	expression tag	UNP A7Y7W1
F	541	HIS	-	expression tag	UNP A7Y7W1
G	536	HIS	-	expression tag	UNP A7Y7W1
G	537	HIS	-	expression tag	UNP A7Y7W1
G	538	HIS	-	expression tag	UNP A7Y7W1
G	539	HIS	-	expression tag	UNP A7Y7W1
G	540	HIS	-	expression tag	UNP A7Y7W1
G	541	HIS	-	expression tag	UNP A7Y7W1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	274	Total O 274 274	0	0
2	A	219	Total O 219 219	0	0

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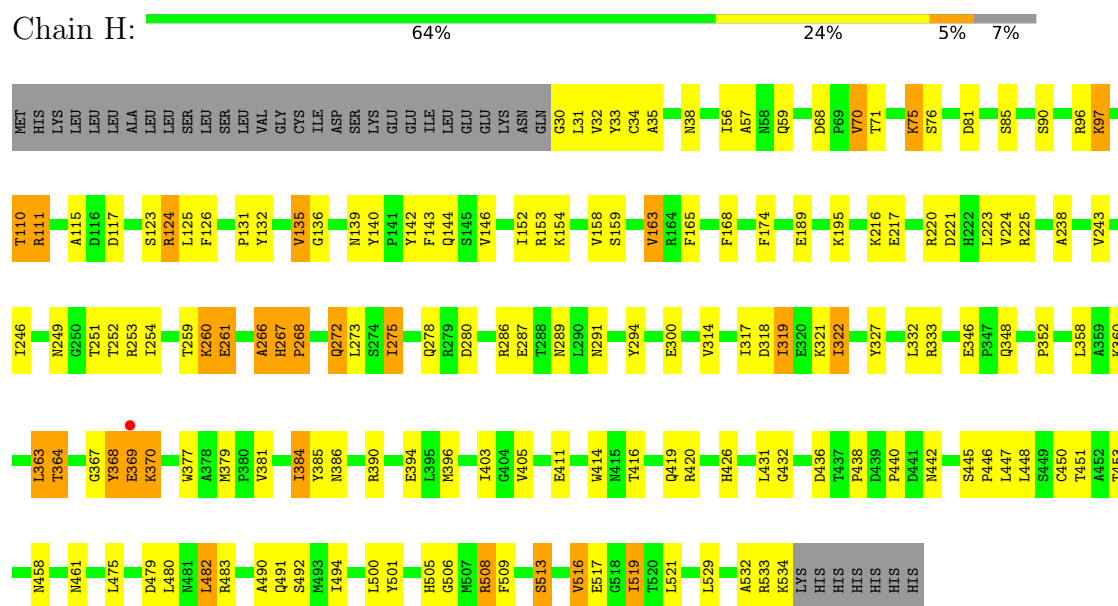
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	225	Total 225	O 225	0	0
2	C	227	Total 227	O 227	0	0
2	D	211	Total 211	O 211	0	0
2	E	159	Total 159	O 159	0	0
2	F	186	Total 186	O 186	0	0
2	G	181	Total 181	O 181	0	0

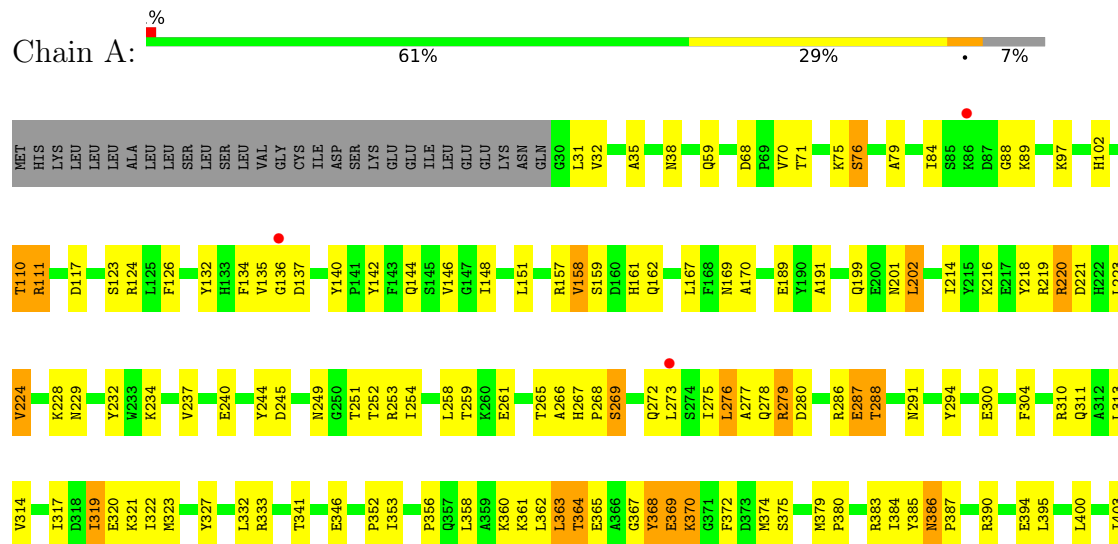
3 Residue-property plots

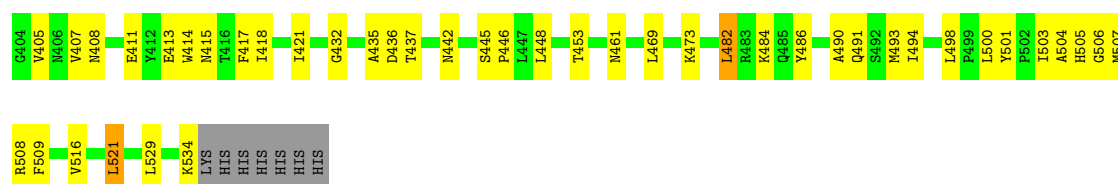
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: ABC transporter periplasmic peptide-binding protein

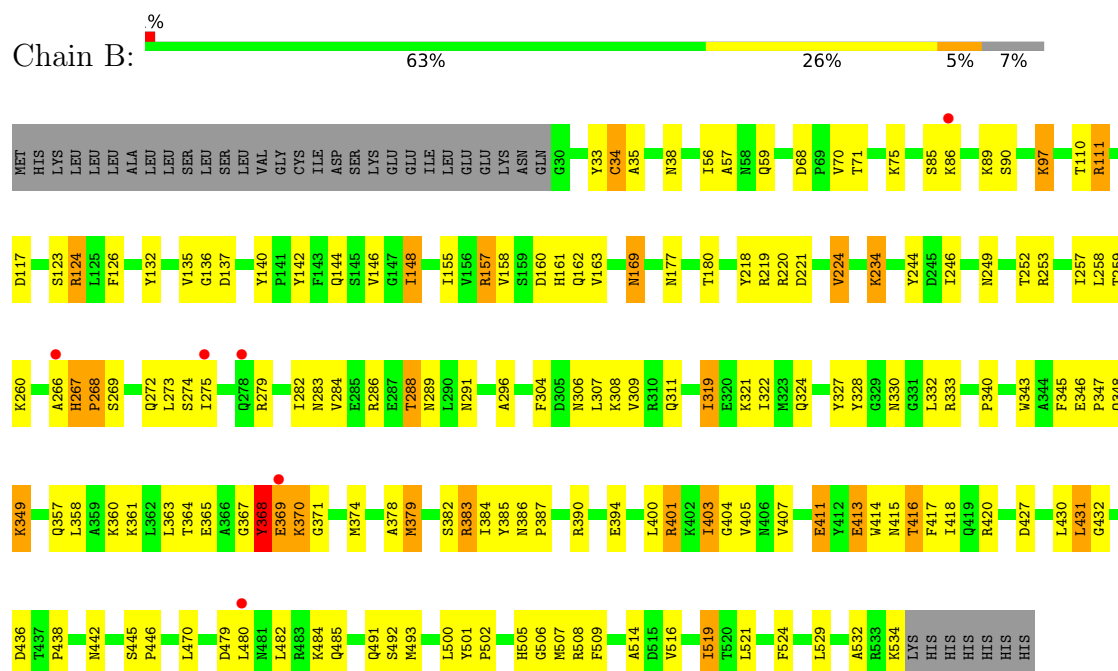


- Molecule 1: ABC transporter periplasmic peptide-binding protein

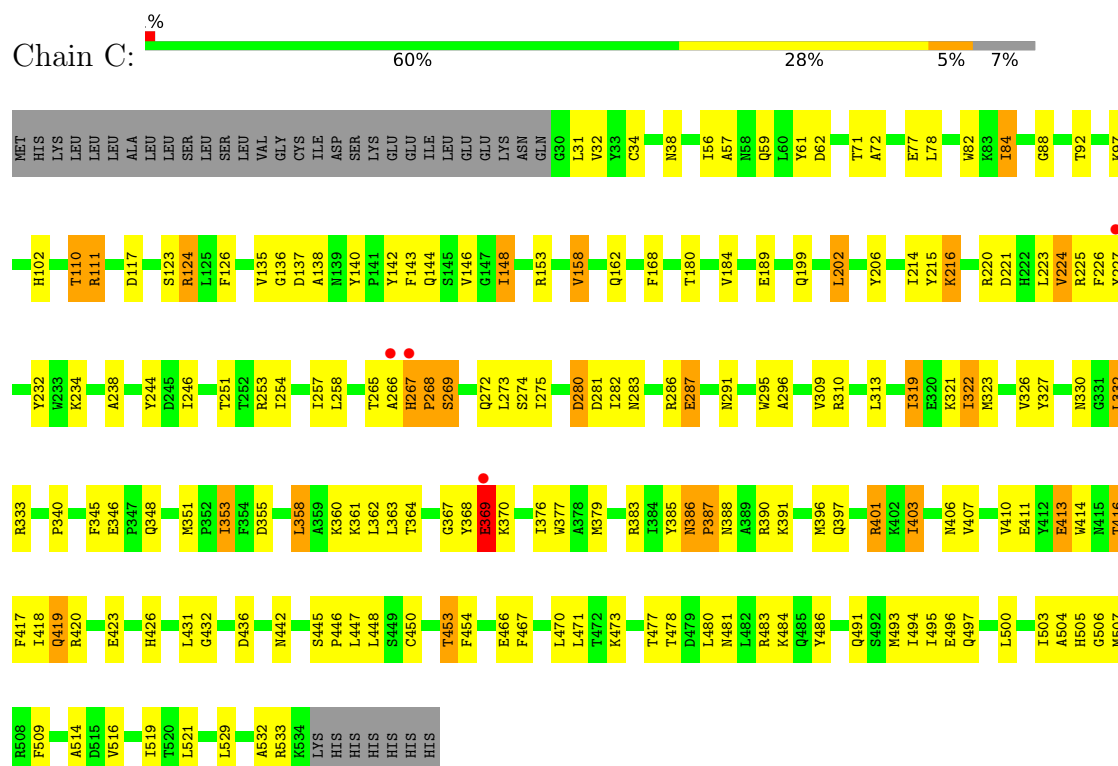




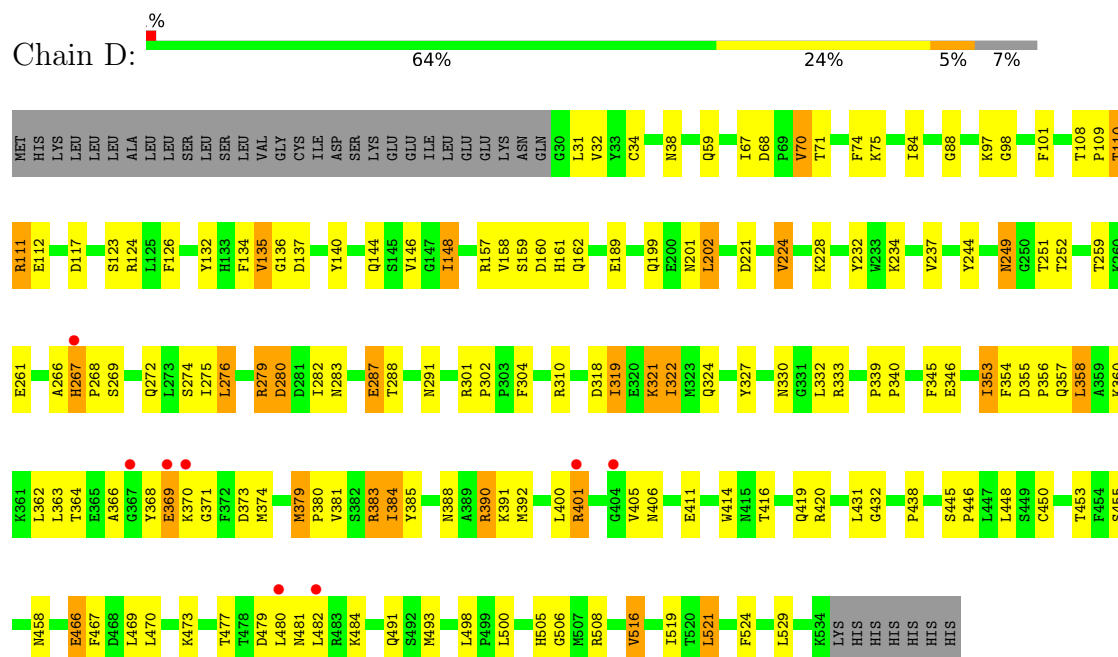
- Molecule 1: ABC transporter periplasmic peptide-binding protein



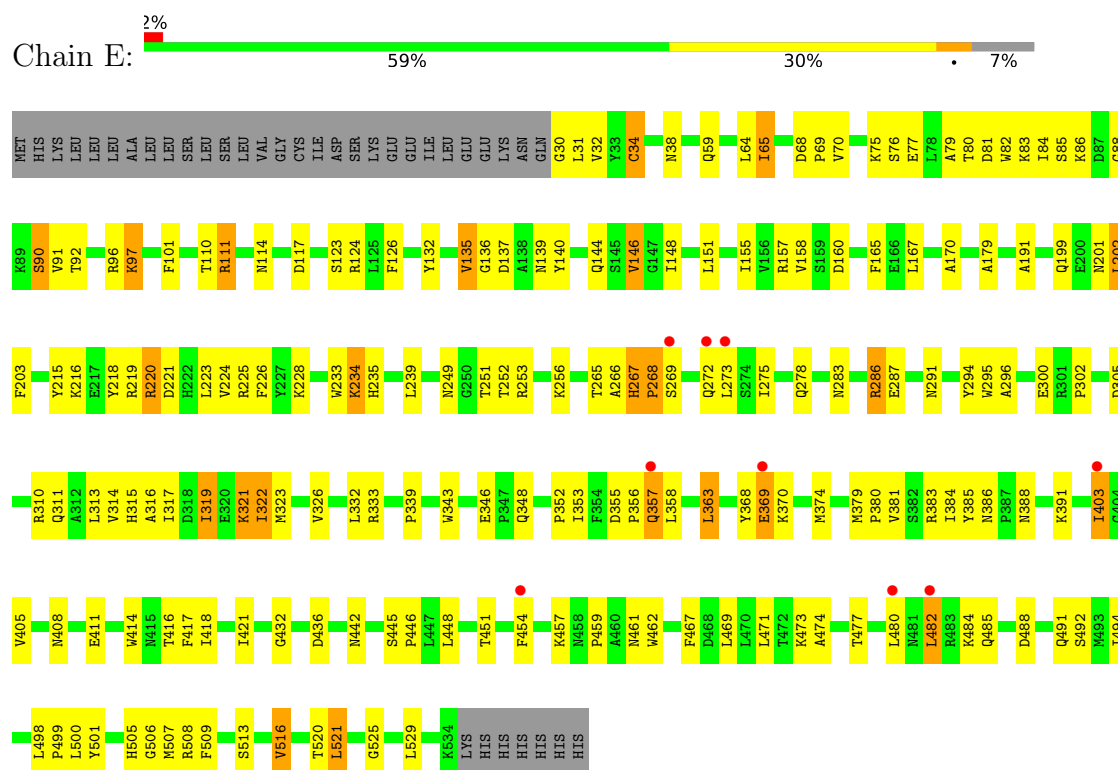
- Molecule 1: ABC transporter periplasmic peptide-binding protein



- Molecule 1: ABC transporter periplasmic peptide-binding protein

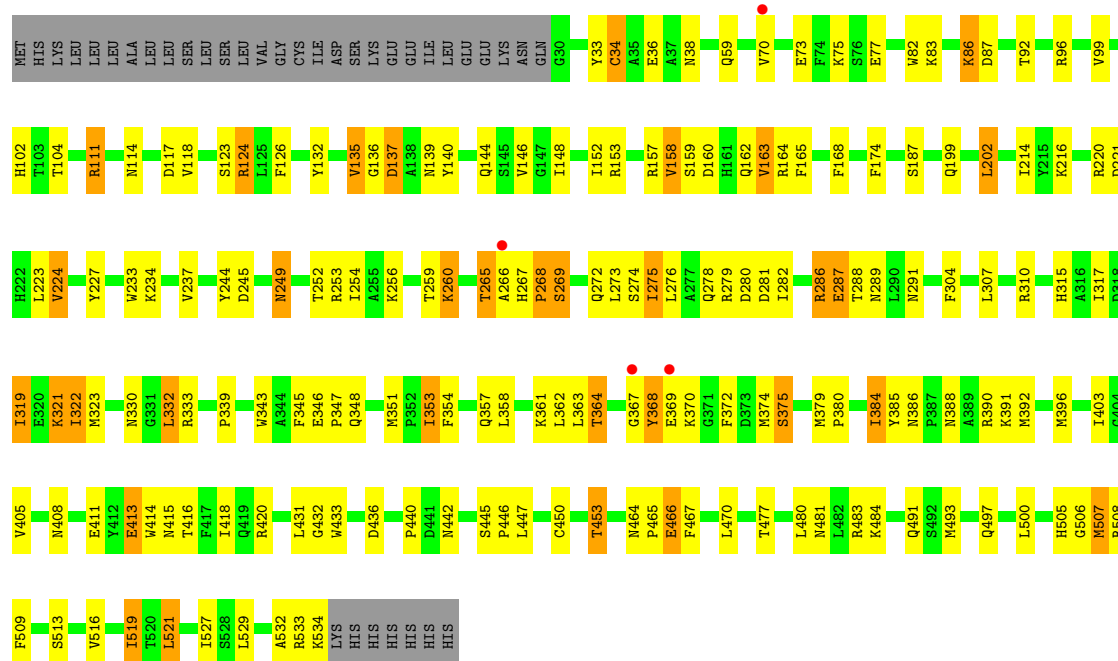


- Molecule 1: ABC transporter periplasmic peptide-binding protein

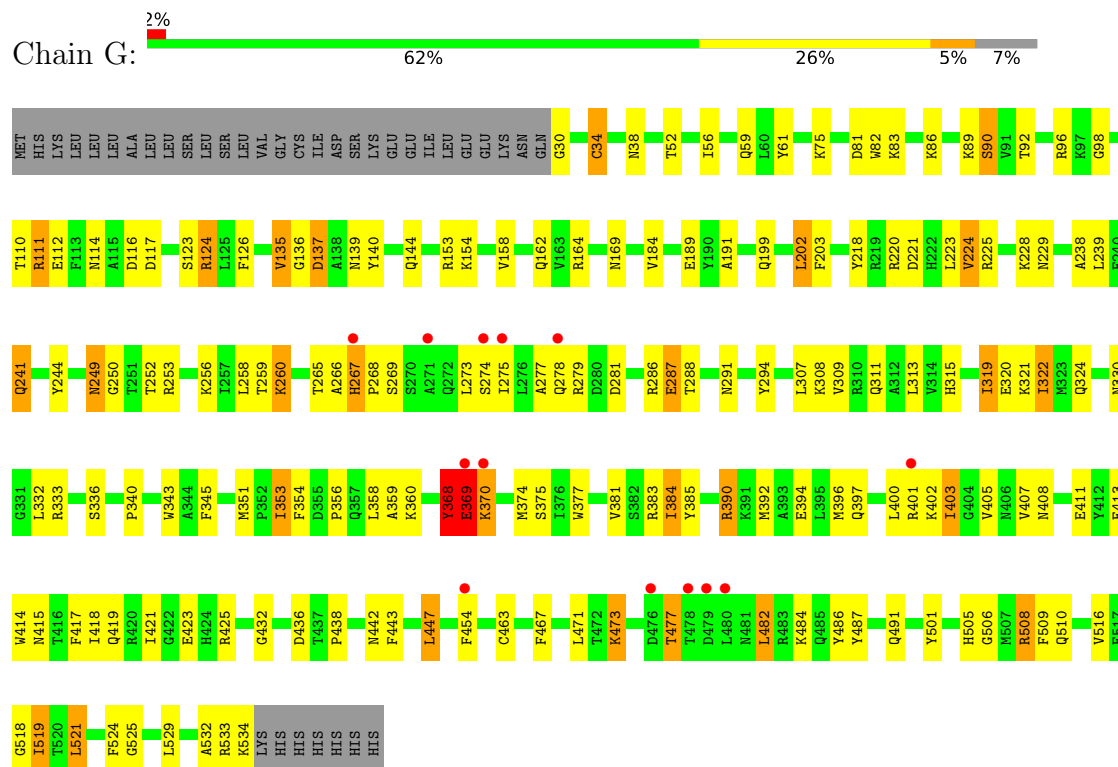


- Molecule 1: ABC transporter periplasmic peptide-binding protein





- Molecule 1: ABC transporter periplasmic peptide-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.39Å 93.97Å 140.55Å 80.03° 84.43° 69.84°	Depositor
Resolution (Å)	42.63 – 2.29 42.63 – 2.29	Depositor EDS
% Data completeness (in resolution range)	88.7 (42.63-2.29) 93.1 (42.63-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.191 , 0.257 0.190 , 0.253	Depositor DCC
R_{free} test set	9375 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34170	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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	0.45	1/4166 (0.0%)	0.61	1/5667 (0.0%)
1	B	0.45	1/4166 (0.0%)	0.62	2/5667 (0.0%)
1	C	0.45	1/4166 (0.0%)	0.62	1/5667 (0.0%)
1	D	0.41	0/4166	0.59	0/5667
1	E	0.40	1/4166 (0.0%)	0.58	1/5667 (0.0%)
1	F	0.39	0/4166	0.58	0/5667
1	G	0.39	0/4166	0.58	0/5667
1	H	0.45	0/4166	0.61	0/5667
All	All	0.42	4/33328 (0.0%)	0.60	5/45336 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	PRO	N-CD	5.35	1.55	1.47
1	C	387	PRO	N-CD	5.35	1.55	1.47
1	E	356	PRO	N-CD	5.28	1.55	1.47
1	B	387	PRO	N-CD	5.24	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	ASN	C-N-CD	5.53	140.02	128.40
1	E	355	ASP	C-N-CD	5.53	140.01	128.40
1	B	386	ASN	C-N-CD	5.51	139.97	128.40
1	C	386	ASN	C-N-CD	5.50	139.96	128.40
1	B	157	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4061	0	3968	164	0
1	B	4061	0	3968	151	0
1	C	4061	0	3968	177	0
1	D	4061	0	3968	145	0
1	E	4061	0	3968	139	0
1	F	4061	0	3968	169	0
1	G	4061	0	3968	136	0
1	H	4061	0	3968	138	0
2	A	219	0	0	10	0
2	B	225	0	0	9	0
2	C	227	0	0	3	0
2	D	211	0	0	5	0
2	E	159	0	0	4	0
2	F	186	0	0	7	0
2	G	181	0	0	3	0
2	H	274	0	0	7	0
All	All	34170	0	31744	1204	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 19.

All (1204) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:275:ILE:HD11	1:C:274:SER:HB2	1.30	1.12
1:D:279:ARG:HB2	1:D:280:ASP:CA	1.76	1.12
1:C:84:ILE:HD11	1:C:88:GLY:HA2	1.27	1.10
1:E:368:TYR:CA	1:E:369:GLU:HB2	1.82	1.09
1:H:384:ILE:HD13	1:H:384:ILE:H	1.12	1.08
1:E:368:TYR:HA	1:E:369:GLU:HB2	1.20	1.07
1:B:368:TYR:HA	1:B:369:GLU:HB2	1.35	1.07
1:D:369:GLU:H	1:D:370:LYS:HA	1.14	1.06
1:G:368:TYR:HA	1:G:369:GLU:HB2	1.36	1.06
1:D:279:ARG:HB2	1:D:280:ASP:HA	1.11	1.06
1:D:368:TYR:HA	1:D:369:GLU:HB2	1.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:GLU:N	1:E:370:LYS:HA	1.71	1.05
1:B:268:PRO:HG2	1:B:273:LEU:HD21	1.40	1.04
1:D:369:GLU:N	1:D:370:LYS:HA	1.68	1.04
1:A:322:ILE:HG22	1:A:395:LEU:HD12	1.39	1.04
1:D:384:ILE:HD13	1:D:384:ILE:H	1.18	1.03
1:F:268:PRO:CB	1:F:272:GLN:HE21	1.71	1.02
1:H:368:TYR:C	1:H:370:LYS:HA	1.79	1.01
1:F:86:LYS:H	1:F:86:LYS:HD3	1.25	1.01
1:F:369:GLU:N	1:F:370:LYS:HA	1.77	1.00
1:A:320:GLU:HB3	1:B:349:LYS:HG3	1.42	0.98
1:A:368:TYR:N	1:A:369:GLU:HB2	1.76	0.98
1:A:369:GLU:N	1:A:370:LYS:HA	1.78	0.98
1:D:291:ASN:HD21	1:D:506:GLY:H	1.03	0.98
1:C:397:GLN:HG2	1:C:401:ARG:HH12	1.30	0.97
1:B:291:ASN:HD21	1:B:506:GLY:H	1.09	0.97
1:B:369:GLU:N	1:B:370:LYS:HA	1.76	0.97
1:G:269:SER:HB2	1:G:330:ASN:HD21	1.30	0.96
1:F:249:ASN:HD22	1:F:252:THR:H	1.14	0.96
1:G:384:ILE:HD13	1:G:384:ILE:H	1.26	0.96
1:B:286:ARG:HH12	1:D:280:ASP:HB2	1.27	0.95
1:C:379:MET:HE1	1:C:386:ASN:HB3	1.49	0.95
1:F:268:PRO:CB	1:F:272:GLN:NE2	2.30	0.94
1:F:319:ILE:O	1:F:322:ILE:HG22	1.66	0.94
1:D:249:ASN:ND2	1:D:252:THR:H	1.66	0.93
1:E:295:TRP:HZ3	1:E:317:ILE:HD11	1.33	0.93
1:E:379:MET:CE	1:E:386:ASN:HB3	1.98	0.93
1:D:279:ARG:CB	1:D:280:ASP:HA	1.99	0.93
1:A:249:ASN:HD22	1:A:252:THR:H	1.17	0.92
1:G:369:GLU:N	1:G:370:LYS:HA	1.84	0.92
1:H:38:ASN:HD21	1:H:221:ASP:H	1.13	0.92
1:G:360:LYS:HZ3	1:G:370:LYS:HB2	1.33	0.91
1:A:379:MET:HE1	1:A:386:ASN:HB3	1.52	0.90
1:A:291:ASN:HD21	1:A:506:GLY:H	1.14	0.90
1:C:38:ASN:HD21	1:C:221:ASP:H	1.18	0.90
1:H:360:LYS:O	1:H:364:THR:HG22	1.70	0.90
1:G:368:TYR:HA	1:G:369:GLU:CB	1.97	0.89
1:G:369:GLU:H	1:G:370:LYS:HA	1.36	0.88
1:F:268:PRO:HB2	1:F:272:GLN:HE21	1.38	0.88
1:H:369:GLU:N	1:H:370:LYS:HA	1.88	0.87
1:F:319:ILE:HG12	1:F:333:ARG:CZ	2.04	0.87
1:C:379:MET:CE	1:C:386:ASN:HB3	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:GLN:HB3	1:E:202:LEU:HD22	1.54	0.87
1:B:401:ARG:HE	1:B:401:ARG:HA	1.39	0.87
1:F:275:ILE:H	1:F:275:ILE:HD12	1.37	0.87
1:G:353:ILE:HD12	1:G:354:PHE:H	1.37	0.86
1:F:77:GLU:O	1:F:96:ARG:NH2	2.09	0.86
1:C:369:GLU:N	1:C:370:LYS:HA	1.90	0.86
1:A:286:ARG:H	1:B:357:GLN:HE22	1.24	0.86
1:F:379:MET:CE	1:F:386:ASN:HB3	2.06	0.86
1:E:295:TRP:CZ3	1:E:317:ILE:HD11	2.11	0.85
1:H:384:ILE:HD13	1:H:384:ILE:N	1.91	0.85
1:G:443:PHE:O	1:G:447:LEU:HD11	1.75	0.85
1:C:216:LYS:HG2	1:C:225:ARG:HD2	1.59	0.85
1:G:291:ASN:HD21	1:G:506:GLY:H	1.23	0.85
1:A:379:MET:CE	1:A:386:ASN:HB3	2.07	0.85
1:C:368:TYR:CA	1:C:369:GLU:HB2	2.05	0.85
1:G:360:LYS:NZ	1:G:370:LYS:HB2	1.92	0.85
1:C:368:TYR:HA	1:C:369:GLU:HB2	1.57	0.84
1:E:249:ASN:HD22	1:E:252:THR:H	1.19	0.84
1:B:249:ASN:HD22	1:B:252:THR:H	1.22	0.84
1:D:384:ILE:H	1:D:384:ILE:CD1	1.87	0.84
1:A:368:TYR:CA	1:A:369:GLU:HB2	2.07	0.84
1:F:268:PRO:HG2	1:F:273:LEU:HD21	1.59	0.84
1:A:384:ILE:HG12	1:A:506:GLY:HA3	1.59	0.84
1:A:414:TRP:CE2	1:A:418:ILE:HD11	2.12	0.84
1:H:419:GLN:HG3	1:H:420:ARG:N	1.93	0.83
1:C:401:ARG:HH21	1:C:406:ASN:HA	1.42	0.83
1:F:86:LYS:H	1:F:86:LYS:CD	1.87	0.83
1:D:384:ILE:HD13	1:D:384:ILE:N	1.94	0.83
1:B:346:GLU:H	1:B:491:GLN:HE22	1.24	0.83
1:C:269:SER:HA	1:C:330:ASN:HD21	1.44	0.82
1:H:314:VAL:HG11	1:H:352:PRO:HG2	1.62	0.82
1:C:401:ARG:NH2	1:C:407:VAL:H	1.76	0.82
1:A:288:THR:HA	2:A:695:HOH:O	1.79	0.82
1:A:360:LYS:NZ	1:A:370:LYS:HG3	1.95	0.82
1:H:291:ASN:O	1:H:505:HIS:HD2	1.63	0.81
1:E:379:MET:HE3	1:E:386:ASN:HB3	1.60	0.81
1:F:291:ASN:HD21	1:F:506:GLY:H	1.26	0.81
1:C:153:ARG:HG3	1:C:168:PHE:CE1	2.15	0.81
1:C:268:PRO:CB	1:C:272:GLN:NE2	2.44	0.81
1:C:291:ASN:HD21	1:C:506:GLY:H	1.23	0.81
1:B:319:ILE:HD11	1:B:333:ARG:CD	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:PRO:HB3	1:F:272:GLN:NE2	1.94	0.81
1:B:416:THR:HG22	1:B:420:ARG:HE	1.45	0.81
1:A:414:TRP:CZ2	1:A:418:ILE:HD11	2.16	0.81
1:A:253:ARG:HB3	1:A:265:THR:HG21	1.63	0.80
1:G:370:LYS:H	1:G:370:LYS:HD2	1.44	0.80
1:A:360:LYS:O	1:A:364:THR:HG22	1.82	0.80
1:H:139:ASN:HD22	1:H:144:GLN:HE22	1.26	0.80
1:A:322:ILE:HG22	1:A:395:LEU:CD1	2.11	0.80
1:B:368:TYR:HA	1:B:369:GLU:CB	2.10	0.80
1:B:273:LEU:HD11	1:B:509:PHE:HB3	1.64	0.80
1:D:368:TYR:CA	1:D:369:GLU:HB2	2.12	0.79
1:A:368:TYR:C	1:A:370:LYS:HA	2.03	0.79
1:D:481:ASN:HA	1:D:484:LYS:HD2	1.65	0.79
1:H:140:TYR:H	1:H:144:GLN:NE2	1.80	0.79
1:B:390:ARG:HH11	1:B:411:GLU:HG3	1.46	0.79
1:C:268:PRO:HB2	1:C:272:GLN:HE21	1.48	0.79
1:C:361:LYS:O	1:C:364:THR:HG22	1.83	0.79
1:G:375:SER:HB3	1:G:408:ASN:OD1	1.83	0.78
1:D:38:ASN:HD21	1:D:221:ASP:H	1.30	0.78
1:C:38:ASN:ND2	1:C:221:ASP:H	1.80	0.78
1:H:38:ASN:ND2	1:H:221:ASP:H	1.80	0.78
1:G:268:PRO:HG2	1:G:273:LEU:HD21	1.64	0.78
1:A:146:VAL:HG13	1:A:148:ILE:HD13	1.66	0.78
1:C:450:CYS:O	1:C:453:THR:HB	1.84	0.78
1:H:59:GLN:NE2	1:H:529:LEU:H	1.82	0.78
1:H:268:PRO:HG2	1:H:273:LEU:HD21	1.66	0.77
1:H:384:ILE:H	1:H:384:ILE:CD1	1.84	0.77
1:F:450:CYS:O	1:F:453:THR:HB	1.83	0.77
1:H:314:VAL:HG13	1:H:501:TYR:CE2	2.20	0.77
1:E:369:GLU:N	1:E:370:LYS:CA	2.48	0.77
1:A:310:ARG:HD3	1:A:498:LEU:O	1.86	0.76
1:G:384:ILE:HD13	1:G:384:ILE:N	2.00	0.76
1:E:38:ASN:HD21	1:E:221:ASP:H	1.31	0.76
1:C:346:GLU:H	1:C:491:GLN:HE22	1.33	0.76
1:A:319:ILE:HD11	1:A:333:ARG:HG3	1.68	0.76
1:E:314:VAL:HG13	1:E:501:TYR:CE2	2.21	0.75
1:F:481:ASN:HA	1:F:484:LYS:HD2	1.67	0.75
1:G:34:CYS:HB3	1:G:253:ARG:HG2	1.65	0.75
1:A:228:LYS:HE3	1:A:237:VAL:O	1.87	0.75
1:D:249:ASN:HD22	1:D:252:THR:H	1.33	0.75
1:H:364:THR:HG21	2:H:755:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:PRO:HD2	1:E:509:PHE:HB2	1.69	0.75
1:H:450:CYS:O	1:H:453:THR:HB	1.86	0.75
1:G:384:ILE:H	1:G:384:ILE:CD1	1.91	0.75
1:C:268:PRO:CG	1:C:509:PHE:HB2	2.17	0.75
1:F:291:ASN:O	1:F:505:HIS:HD2	1.70	0.74
1:D:360:LYS:HZ2	1:D:370:LYS:HB2	1.50	0.74
1:B:140:TYR:H	1:B:144:GLN:NE2	1.85	0.74
1:H:289:ASN:HB2	1:H:508:ARG:HG2	1.69	0.74
1:A:507:MET:HA	2:A:695:HOH:O	1.88	0.74
1:F:368:TYR:C	1:F:370:LYS:HA	2.08	0.74
1:E:291:ASN:HD21	1:E:506:GLY:H	1.36	0.74
1:H:319:ILE:HA	1:H:322:ILE:CG2	2.17	0.74
1:F:519:ILE:HD13	1:F:532:ALA:HB2	1.70	0.74
1:G:140:TYR:H	1:G:144:GLN:NE2	1.86	0.74
1:D:368:TYR:HA	1:D:369:GLU:CB	2.06	0.74
1:C:322:ILE:HD13	1:C:323:MET:N	2.02	0.73
1:F:289:ASN:HD22	1:F:508:ARG:HH11	1.35	0.73
1:C:268:PRO:HB2	1:C:272:GLN:NE2	2.01	0.73
1:E:30:GLY:N	2:E:722:HOH:O	2.21	0.73
1:H:368:TYR:N	1:H:369:GLU:HB2	2.03	0.73
1:C:199:GLN:HB3	1:C:202:LEU:HD22	1.71	0.73
1:G:368:TYR:CA	1:G:369:GLU:HB2	2.15	0.73
1:G:390:ARG:HH12	1:G:411:GLU:HB3	1.51	0.73
1:C:397:GLN:HG2	1:C:401:ARG:NH1	2.02	0.73
1:E:249:ASN:ND2	1:E:252:THR:H	1.87	0.73
1:H:153:ARG:HG3	1:H:168:PHE:CE1	2.24	0.73
1:F:372:PHE:HE1	1:F:374:MET:HE2	1.52	0.73
1:F:379:MET:HE1	1:F:386:ASN:HB3	1.71	0.72
1:B:390:ARG:O	1:B:394:GLU:HG3	1.90	0.72
1:D:199:GLN:HB3	1:D:202:LEU:HD22	1.69	0.72
1:E:368:TYR:C	1:E:370:LYS:HA	2.09	0.72
1:B:370:LYS:H	1:B:370:LYS:HD2	1.55	0.72
1:B:266:ALA:O	1:B:267:HIS:O	2.07	0.72
1:F:321:LYS:HD3	1:F:321:LYS:O	1.89	0.72
1:G:353:ILE:HD12	1:G:354:PHE:N	2.04	0.72
1:B:411:GLU:HA	2:B:642:HOH:O	1.89	0.72
1:D:369:GLU:N	1:D:370:LYS:CA	2.49	0.72
1:F:38:ASN:HD21	1:F:221:ASP:H	1.37	0.71
1:D:291:ASN:O	1:D:505:HIS:HD2	1.72	0.71
1:E:322:ILE:HD13	1:E:322:ILE:C	2.10	0.71
1:G:269:SER:CB	1:G:330:ASN:HD21	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:TYR:H	1:D:144:GLN:NE2	1.89	0.71
1:F:216:LYS:HB2	1:F:227:TYR:HD2	1.56	0.71
1:D:59:GLN:NE2	1:D:529:LEU:H	1.88	0.71
1:G:199:GLN:HB3	1:G:202:LEU:HD22	1.71	0.71
1:F:353:ILE:HD13	1:F:354:PHE:H	1.56	0.70
1:A:356:PRO:O	1:A:403:ILE:HD11	1.92	0.70
1:A:278:GLN:HA	1:A:279:ARG:C	2.11	0.70
1:F:249:ASN:ND2	1:F:252:THR:H	1.86	0.70
1:E:220:ARG:CD	1:E:220:ARG:H	2.04	0.70
1:A:110:THR:HB	1:A:189:GLU:OE2	1.92	0.70
1:C:158:VAL:HG13	1:C:162:GLN:HB3	1.71	0.70
1:G:279:ARG:HB3	1:G:281:ASP:OD1	1.91	0.69
1:F:137:ASP:OD1	1:F:137:ASP:N	2.25	0.69
1:H:85:SER:HB3	1:H:90:SER:HB2	1.74	0.69
1:D:353:ILE:HD13	1:D:354:PHE:H	1.56	0.69
1:G:291:ASN:O	1:G:505:HIS:HD2	1.75	0.69
1:B:269:SER:HB2	1:B:330:ASN:HD21	1.56	0.69
1:F:140:TYR:H	1:F:144:GLN:HE21	1.39	0.69
1:G:258:LEU:HD22	1:G:279:ARG:HH12	1.58	0.69
1:F:199:GLN:HB3	1:F:202:LEU:HD22	1.74	0.69
1:F:379:MET:HE3	1:F:386:ASN:HB3	1.75	0.69
1:H:68:ASP:HB2	1:H:75:LYS:HG3	1.74	0.69
1:A:38:ASN:HD21	1:A:221:ASP:H	1.39	0.69
1:A:505:HIS:HE1	2:A:762:HOH:O	1.75	0.69
1:D:431:LEU:HG	1:D:432:GLY:H	1.57	0.69
1:E:343:TRP:HE3	1:E:484:LYS:HE2	1.58	0.68
1:G:111:ARG:NH2	1:G:117:ASP:OD2	2.26	0.68
1:H:225:ARG:HD2	1:H:243:VAL:HG22	1.75	0.68
1:A:353:ILE:HG12	2:A:723:HOH:O	1.94	0.68
1:H:249:ASN:HD22	1:H:252:THR:H	1.40	0.68
1:B:384:ILE:HG12	1:B:506:GLY:HA3	1.76	0.68
1:B:368:TYR:CA	1:B:369:GLU:HB2	2.19	0.68
1:B:157:ARG:NH2	1:B:160:ASP:OD1	2.26	0.68
1:B:401:ARG:NH2	1:B:407:VAL:H	1.92	0.68
1:B:416:THR:CG2	1:B:420:ARG:HE	2.07	0.68
1:C:367:GLY:C	1:C:369:GLU:HB2	2.14	0.68
1:H:346:GLU:H	1:H:491:GLN:HE22	1.40	0.68
1:A:249:ASN:ND2	1:A:252:THR:H	1.89	0.68
1:C:269:SER:HA	1:C:330:ASN:ND2	2.08	0.68
1:G:319:ILE:HG21	1:G:333:ARG:NE	2.08	0.68
1:A:368:TYR:CA	1:A:369:GLU:CB	2.72	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ARG:HB3	1:C:265:THR:HG21	1.74	0.67
1:D:279:ARG:HB3	1:D:282:ILE:H	1.57	0.67
1:B:33:TYR:CE1	1:B:266:ALA:HB2	2.29	0.67
1:C:269:SER:CA	1:C:330:ASN:HD21	2.08	0.67
1:F:124:ARG:HD3	1:F:132:TYR:O	1.93	0.67
1:H:259:THR:C	1:H:260:LYS:HD3	2.15	0.67
1:D:467:PHE:HA	1:D:493:MET:CE	2.25	0.67
1:B:360:LYS:NZ	1:B:370:LYS:HG3	2.10	0.67
1:F:123:SER:HA	1:F:126:PHE:CE2	2.30	0.67
1:F:233:TRP:CZ3	1:F:234:LYS:HB2	2.29	0.67
1:C:38:ASN:HD21	1:C:221:ASP:N	1.90	0.67
1:D:479:ASP:HB3	1:D:482:LEU:HD12	1.76	0.67
1:H:451:THR:HG23	2:H:723:HOH:O	1.94	0.66
1:E:59:GLN:NE2	1:E:529:LEU:H	1.93	0.66
1:D:360:LYS:NZ	1:D:370:LYS:HB2	2.10	0.66
1:F:374:MET:SD	2:F:714:HOH:O	2.54	0.66
1:H:436:ASP:H	1:H:442:ASN:ND2	1.94	0.66
1:A:369:GLU:N	1:A:370:LYS:CA	2.57	0.66
1:D:279:ARG:CB	1:D:280:ASP:CA	2.61	0.66
1:G:224:VAL:HG13	1:G:244:TYR:HB2	1.78	0.66
1:G:374:MET:CE	1:G:400:LEU:HD13	2.25	0.66
1:H:369:GLU:N	1:H:370:LYS:CA	2.59	0.66
1:G:38:ASN:HD21	1:G:221:ASP:H	1.44	0.66
1:E:140:TYR:H	1:E:144:GLN:NE2	1.93	0.66
1:F:445:SER:HB2	1:F:446:PRO:HD3	1.78	0.66
1:H:70:VAL:HG22	1:H:71:THR:HG23	1.76	0.65
1:F:268:PRO:HD2	1:F:509:PHE:HB2	1.77	0.65
1:F:319:ILE:HG21	1:F:333:ARG:NH2	2.10	0.65
1:H:38:ASN:HD21	1:H:221:ASP:N	1.90	0.65
1:B:234:LYS:HE3	2:B:731:HOH:O	1.96	0.65
1:B:137:ASP:HA	2:B:664:HOH:O	1.96	0.65
1:E:300:GLU:HB2	1:E:461:ASN:ND2	2.12	0.65
1:E:368:TYR:N	1:E:369:GLU:HB2	2.10	0.65
1:D:110:THR:HB	1:D:189:GLU:OE2	1.96	0.65
1:B:369:GLU:H	1:B:370:LYS:HA	1.58	0.65
1:G:269:SER:HB2	1:G:330:ASN:ND2	2.09	0.65
1:F:157:ARG:HH21	1:F:159:SER:HA	1.61	0.65
1:C:254:ILE:CD1	1:C:272:GLN:HB3	2.27	0.65
1:C:319:ILE:O	1:C:323:MET:HG2	1.96	0.65
1:F:140:TYR:H	1:F:144:GLN:NE2	1.94	0.65
1:F:275:ILE:H	1:F:275:ILE:CD1	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:322:ILE:HD11	1:H:327:TYR:HE1	1.62	0.65
1:C:84:ILE:CD1	1:C:88:GLY:HA2	2.18	0.65
1:A:266:ALA:O	1:A:268:PRO:HD3	1.96	0.64
1:B:275:ILE:HD12	1:B:275:ILE:H	1.62	0.64
1:B:291:ASN:O	1:B:505:HIS:HD2	1.80	0.64
1:F:33:TYR:HE1	1:F:266:ALA:HB2	1.62	0.64
1:F:157:ARG:O	1:F:157:ARG:HG3	1.95	0.64
1:E:368:TYR:CA	1:E:369:GLU:CB	2.68	0.64
1:C:322:ILE:HD13	1:C:322:ILE:C	2.19	0.64
1:F:158:VAL:HG21	1:F:162:GLN:OE1	1.98	0.64
1:B:364:THR:HA	1:B:367:GLY:O	1.97	0.64
1:C:367:GLY:O	1:C:369:GLU:HB2	1.97	0.64
1:F:390:ARG:HH21	1:F:411:GLU:HB2	1.62	0.63
1:B:286:ARG:NH1	1:D:280:ASP:HB2	2.07	0.63
1:A:146:VAL:CG1	1:A:148:ILE:HD13	2.27	0.63
1:B:361:LYS:O	1:B:365:GLU:HG3	1.97	0.63
1:C:466:GLU:HG3	2:C:767:HOH:O	1.97	0.63
1:B:343:TRP:HE3	1:B:484:LYS:HE3	1.63	0.63
1:C:436:ASP:H	1:C:442:ASN:ND2	1.95	0.63
1:H:268:PRO:HD2	1:H:509:PHE:HB2	1.79	0.63
1:H:379:MET:HE3	1:H:386:ASN:HB3	1.80	0.63
1:C:346:GLU:OE1	1:C:484:LYS:NZ	2.31	0.63
1:F:319:ILE:HG12	1:F:333:ARG:NE	2.12	0.63
1:G:191:ALA:HB2	1:G:203:PHE:CE1	2.34	0.63
1:A:368:TYR:HA	1:A:369:GLU:CB	2.28	0.63
1:C:268:PRO:CD	1:C:509:PHE:HB2	2.28	0.63
1:D:97:LYS:HE3	1:D:161:HIS:NE2	2.14	0.63
1:E:311:GLN:O	1:E:315:HIS:CD2	2.51	0.63
1:F:384:ILE:HD13	1:F:384:ILE:H	1.64	0.63
1:F:519:ILE:HD11	1:F:529:LEU:HD23	1.79	0.63
1:A:390:ARG:O	1:A:394:GLU:HG3	1.98	0.63
1:C:319:ILE:O	1:C:319:ILE:HG13	1.99	0.63
1:C:473:LYS:HD3	1:C:486:TYR:CE1	2.33	0.63
1:E:146:VAL:HG13	1:E:148:ILE:HD13	1.80	0.63
1:G:419:GLN:O	1:G:423:GLU:HG3	1.99	0.63
1:C:388:ASN:ND2	1:C:391:LYS:HB2	2.13	0.62
1:D:319:ILE:HG12	1:D:333:ARG:CZ	2.29	0.62
1:E:68:ASP:OD1	1:E:69:PRO:HD2	1.98	0.62
1:C:368:TYR:HA	1:C:369:GLU:CB	2.26	0.62
1:D:158:VAL:HG22	1:D:162:GLN:O	1.99	0.62
1:F:59:GLN:NE2	1:F:529:LEU:H	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ILE:HD11	1:C:88:GLY:CA	2.16	0.62
1:C:269:SER:HB2	1:C:330:ASN:HD21	1.64	0.62
1:F:321:LYS:HD3	1:F:321:LYS:C	2.19	0.62
1:H:152:ILE:HD11	1:H:174:PHE:HE1	1.65	0.62
1:A:368:TYR:HA	1:A:369:GLU:HB2	1.79	0.62
1:C:467:PHE:CE2	1:C:494:ILE:HD11	2.35	0.62
1:G:90:SER:OG	1:G:164:ARG:HD2	1.99	0.62
1:G:220:ARG:HD2	1:G:221:ASP:OD2	1.99	0.62
1:F:372:PHE:HE1	1:F:374:MET:CE	2.11	0.62
1:H:319:ILE:HD11	1:H:333:ARG:HG3	1.82	0.61
1:C:124:ARG:HD3	1:C:140:TYR:OH	1.99	0.61
1:F:287:GLU:HB2	1:F:521:LEU:HD13	1.81	0.61
1:H:249:ASN:HD21	1:H:251:THR:HB	1.64	0.61
1:B:33:TYR:HE1	1:B:266:ALA:HB2	1.63	0.61
1:D:224:VAL:HG13	1:D:244:TYR:HB2	1.81	0.61
1:F:288:THR:HG21	1:F:332:LEU:HD12	1.82	0.61
1:A:258:LEU:CD2	1:A:279:ARG:HE	2.14	0.61
1:B:401:ARG:HE	1:B:401:ARG:CA	2.10	0.61
1:G:519:ILE:HD11	1:G:532:ALA:HB2	1.80	0.61
1:H:139:ASN:ND2	1:H:144:GLN:HE22	1.97	0.61
1:H:322:ILE:C	1:H:322:ILE:HD13	2.21	0.61
1:H:153:ARG:HG3	1:H:168:PHE:CZ	2.36	0.61
1:H:314:VAL:CG1	1:H:352:PRO:HG2	2.29	0.61
1:F:33:TYR:CE1	1:F:266:ALA:HB2	2.35	0.61
1:B:288:THR:HA	1:B:507:MET:HG2	1.83	0.61
1:E:249:ASN:HD21	1:E:251:THR:HB	1.66	0.61
1:E:381:VAL:HG21	1:E:383:ARG:HH21	1.65	0.61
1:D:279:ARG:HB2	1:D:280:ASP:C	2.21	0.61
1:C:327:TYR:O	1:C:330:ASN:HB2	2.01	0.61
1:B:390:ARG:NH1	1:B:411:GLU:HG3	2.15	0.60
1:D:68:ASP:OD1	1:D:70:VAL:HG13	2.01	0.60
1:H:436:ASP:H	1:H:442:ASN:HD21	1.49	0.60
1:B:401:ARG:HA	1:B:401:ARG:NE	2.11	0.60
1:E:385:TYR:CD1	1:E:432:GLY:HA3	2.37	0.60
1:H:480:LEU:HA	1:H:483:ARG:HD2	1.83	0.60
1:F:480:LEU:HD23	1:F:483:ARG:HD2	1.83	0.60
1:C:268:PRO:HG3	1:C:509:PHE:HB2	1.84	0.60
1:D:450:CYS:O	1:D:453:THR:HB	2.02	0.60
1:E:417:PHE:O	1:E:421:ILE:HG12	2.02	0.60
1:A:151:LEU:HD11	1:A:167:LEU:HB3	1.82	0.60
1:F:86:LYS:HD3	1:F:86:LYS:N	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:225:ARG:HG3	1:H:225:ARG:HH11	1.67	0.60
1:F:403:ILE:HG22	1:F:405:VAL:HG23	1.83	0.60
1:D:369:GLU:H	1:D:370:LYS:CA	2.01	0.59
1:D:505:HIS:HE1	2:D:653:HOH:O	1.84	0.59
1:G:38:ASN:ND2	1:G:221:ASP:H	1.99	0.59
1:C:153:ARG:HG3	1:C:168:PHE:CZ	2.36	0.59
1:E:343:TRP:CE3	1:E:484:LYS:HE2	2.37	0.59
1:F:304:PHE:HE1	1:F:374:MET:HE1	1.68	0.59
1:G:238:ALA:HB1	1:G:533:ARG:HG3	1.85	0.59
1:F:118:VAL:HG11	1:F:163:VAL:HG11	1.84	0.59
1:F:164:ARG:HD3	2:F:633:HOH:O	2.02	0.59
1:H:254:ILE:HG13	1:H:272:GLN:HB3	1.85	0.59
1:A:68:ASP:HB2	1:A:75:LYS:CG	2.32	0.59
1:F:86:LYS:HE2	1:F:87:ASP:N	2.17	0.59
1:F:346:GLU:H	1:F:491:GLN:HE22	1.50	0.59
1:C:368:TYR:N	1:C:369:GLU:HB2	2.17	0.59
1:F:34:CYS:HB3	1:F:253:ARG:HG2	1.84	0.59
1:F:86:LYS:CD	1:F:86:LYS:N	2.62	0.59
1:G:59:GLN:NE2	1:G:529:LEU:H	2.00	0.59
1:A:319:ILE:HG12	1:A:333:ARG:NH2	2.18	0.59
1:C:281:ASP:O	1:C:282:ILE:HD13	2.02	0.59
1:H:223:LEU:C	1:H:223:LEU:HD12	2.23	0.59
1:B:258:LEU:HD23	1:B:279:ARG:NH1	2.17	0.59
1:F:275:ILE:HD12	1:F:275:ILE:N	2.15	0.59
1:F:369:GLU:N	1:F:370:LYS:CA	2.60	0.59
1:C:224:VAL:HG13	1:C:244:TYR:HB2	1.84	0.58
1:D:467:PHE:HA	1:D:493:MET:HE1	1.85	0.58
1:G:223:LEU:HD12	1:G:223:LEU:C	2.23	0.58
1:H:363:LEU:O	1:H:367:GLY:O	2.20	0.58
1:D:279:ARG:HG2	1:D:282:ILE:O	2.03	0.58
1:F:86:LYS:HE2	1:F:87:ASP:H	1.68	0.58
1:F:519:ILE:CD1	1:F:532:ALA:HB2	2.33	0.58
1:A:158:VAL:CG2	1:A:162:GLN:HG2	2.33	0.58
1:F:268:PRO:CG	1:F:273:LEU:HD21	2.32	0.58
1:E:76:SER:OG	1:E:79:ALA:O	2.17	0.58
1:A:372:PHE:HE1	1:A:374:MET:HE2	1.69	0.58
1:D:249:ASN:HD22	1:D:249:ASN:C	2.06	0.58
1:F:390:ARG:NH2	1:F:411:GLU:HB2	2.18	0.58
1:F:416:THR:HG22	1:F:420:ARG:NE	2.18	0.58
1:G:390:ARG:HH12	1:G:411:GLU:CB	2.16	0.58
1:A:275:ILE:H	1:A:275:ILE:HD12	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:ARG:HG2	1:F:286:ARG:O	2.03	0.58
1:G:390:ARG:NH1	1:G:411:GLU:HB3	2.19	0.58
1:A:111:ARG:NH2	1:A:117:ASP:OD2	2.37	0.58
1:A:385:TYR:CD1	1:A:432:GLY:HA3	2.39	0.58
1:F:268:PRO:CA	1:F:272:GLN:NE2	2.65	0.58
1:F:363:LEU:O	1:F:367:GLY:O	2.21	0.58
1:B:34:CYS:HB3	1:B:253:ARG:HG2	1.86	0.58
1:B:401:ARG:CA	1:B:401:ARG:NE	2.66	0.58
1:A:314:VAL:HG13	1:A:501:TYR:CE2	2.38	0.58
1:C:111:ARG:NH2	1:C:117:ASP:OD2	2.37	0.58
1:A:38:ASN:ND2	1:A:221:ASP:H	2.02	0.57
1:A:259:THR:OG1	1:A:261:GLU:HG3	2.04	0.57
1:G:158:VAL:HG22	1:G:162:GLN:HB3	1.85	0.57
1:E:368:TYR:HA	1:E:369:GLU:CB	2.13	0.57
1:E:436:ASP:H	1:E:442:ASN:HD21	1.52	0.57
1:A:291:ASN:O	1:A:505:HIS:HD2	1.87	0.57
1:B:224:VAL:HG13	1:B:244:TYR:HB2	1.86	0.57
1:D:158:VAL:CG2	1:D:162:GLN:HB3	2.34	0.57
1:G:374:MET:HE3	1:G:400:LEU:HD13	1.85	0.57
1:A:311:GLN:HG3	2:A:799:HOH:O	2.04	0.57
1:B:360:LYS:HZ1	1:B:370:LYS:HG3	1.68	0.57
1:E:220:ARG:H	1:E:220:ARG:NE	2.03	0.57
1:E:286:ARG:HG3	1:E:286:ARG:HH11	1.70	0.57
1:E:381:VAL:HG21	1:E:383:ARG:NH2	2.20	0.57
1:F:339:PRO:HB3	1:F:505:HIS:CD2	2.40	0.57
1:F:467:PHE:HA	1:F:493:MET:CE	2.34	0.57
1:H:370:LYS:HE2	1:H:370:LYS:O	2.04	0.57
1:F:223:LEU:HD12	1:F:223:LEU:O	2.05	0.57
1:G:351:MET:CE	1:G:501:TYR:HE1	2.18	0.57
1:G:505:HIS:HE1	2:G:604:HOH:O	1.86	0.57
1:A:482:LEU:HD22	1:A:486:TYR:CE2	2.40	0.57
1:C:416:THR:HG22	1:C:420:ARG:HE	1.70	0.57
1:E:76:SER:OG	1:E:80:THR:HA	2.04	0.57
1:E:146:VAL:CG1	1:E:148:ILE:HD13	2.34	0.57
1:B:158:VAL:HG22	1:B:162:GLN:HB3	1.85	0.57
1:B:268:PRO:HD2	1:B:509:PHE:HB2	1.85	0.57
1:A:59:GLN:NE2	1:A:529:LEU:H	2.03	0.57
1:C:254:ILE:HD11	1:C:272:GLN:HB3	1.87	0.57
1:D:232:TYR:CE2	1:D:234:LYS:HB3	2.39	0.57
1:D:385:TYR:CD1	1:D:432:GLY:HA3	2.40	0.57
1:B:374:MET:HE3	1:B:400:LEU:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:123:SER:HA	1:H:126:PHE:CE2	2.40	0.56
1:H:314:VAL:HG13	1:H:501:TYR:CD2	2.40	0.56
1:H:480:LEU:HD23	1:H:483:ARG:HD2	1.87	0.56
1:A:304:PHE:HE1	1:A:374:MET:HE2	1.69	0.56
1:E:467:PHE:CE2	1:E:471:LEU:HD11	2.40	0.56
1:C:416:THR:CG2	1:C:420:ARG:HE	2.18	0.56
1:F:519:ILE:HD11	1:F:529:LEU:CD2	2.34	0.56
1:G:351:MET:HE1	1:G:501:TYR:CE1	2.41	0.56
1:B:59:GLN:NE2	1:B:529:LEU:H	2.03	0.56
1:D:38:ASN:ND2	1:D:221:ASP:H	1.99	0.56
1:E:321:LYS:HD3	1:E:321:LYS:C	2.25	0.56
1:F:310:ARG:NH1	1:F:497:GLN:O	2.37	0.56
1:A:76:SER:HB2	1:A:79:ALA:O	2.05	0.56
1:C:31:LEU:HD23	1:C:32:VAL:N	2.20	0.56
1:C:110:THR:HB	1:C:189:GLU:OE2	2.05	0.56
1:E:296:ALA:HA	1:E:500:LEU:HA	1.87	0.56
1:A:253:ARG:HD2	1:A:265:THR:CG2	2.36	0.56
1:B:346:GLU:N	1:B:491:GLN:HE22	1.98	0.56
1:D:390:ARG:NH1	1:D:411:GLU:HB2	2.21	0.56
1:F:384:ILE:H	1:F:384:ILE:CD1	2.18	0.56
1:A:469:LEU:HG	1:A:473:LYS:HD2	1.88	0.56
1:B:273:LEU:HD13	1:B:284:VAL:HG13	1.87	0.56
1:B:343:TRP:CE3	1:B:484:LYS:HE3	2.41	0.56
1:C:59:GLN:NE2	1:C:529:LEU:H	2.02	0.56
1:C:269:SER:CB	1:C:330:ASN:HD21	2.18	0.56
1:D:379:MET:HE2	1:D:431:LEU:HA	1.88	0.56
1:G:374:MET:CE	1:G:405:VAL:HG11	2.36	0.56
1:H:152:ILE:HD12	1:H:165:PHE:HD2	1.70	0.56
1:A:134:PHE:CZ	1:C:410:VAL:HG13	2.40	0.56
1:F:254:ILE:HD12	1:F:276:LEU:HD11	1.88	0.56
1:F:272:GLN:O	1:F:275:ILE:HD13	2.05	0.56
1:C:355:ASP:OD2	1:C:358:LEU:HB2	2.05	0.56
1:C:431:LEU:HG	1:C:432:GLY:H	1.71	0.56
1:D:275:ILE:HG22	1:D:276:LEU:HD23	1.88	0.56
1:E:291:ASN:HD21	1:E:506:GLY:N	2.02	0.56
1:A:158:VAL:HG22	1:A:162:GLN:HG2	1.87	0.55
1:F:158:VAL:HG22	1:F:162:GLN:HB3	1.88	0.55
1:F:265:THR:HG22	2:F:725:HOH:O	2.05	0.55
1:G:228:LYS:HB2	1:G:239:LEU:O	2.06	0.55
1:G:385:TYR:CD1	1:G:432:GLY:HA3	2.41	0.55
1:G:436:ASP:H	1:G:442:ASN:ND2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ASP:OD1	1:B:70:VAL:HG22	2.07	0.55
1:E:457:LYS:HE2	2:E:652:HOH:O	2.07	0.55
1:A:320:GLU:HB3	1:B:349:LYS:CG	2.27	0.55
1:C:268:PRO:CG	1:C:273:LEU:HD11	2.37	0.55
1:H:317:ILE:HD12	1:H:396:MET:HG2	1.89	0.55
1:D:157:ARG:NH2	1:D:160:ASP:OD1	2.37	0.55
1:D:401:ARG:HB2	1:D:401:ARG:HH11	1.71	0.55
1:E:291:ASN:O	1:E:505:HIS:HD2	1.89	0.55
1:F:216:LYS:HB2	1:F:227:TYR:CD2	2.40	0.55
1:F:259:THR:O	1:F:260:LYS:HB2	2.06	0.55
1:F:322:ILE:CD1	1:F:392:MET:HE2	2.36	0.55
1:F:358:LEU:O	1:F:362:LEU:HG	2.06	0.55
1:H:490:ALA:O	1:H:494:ILE:HG12	2.07	0.55
1:A:254:ILE:HG23	1:A:276:LEU:HD11	1.87	0.55
1:B:436:ASP:H	1:B:442:ASN:ND2	2.03	0.55
1:B:479:ASP:HB3	1:B:482:LEU:HG	1.88	0.55
1:C:224:VAL:HG12	1:C:246:ILE:HD11	1.88	0.55
1:D:390:ARG:HD2	1:D:411:GLU:OE1	2.07	0.55
1:G:319:ILE:HG21	1:G:333:ARG:CZ	2.36	0.55
1:D:321:LYS:HZ2	1:D:321:LYS:HA	1.72	0.55
1:F:390:ARG:NH2	1:F:411:GLU:CB	2.69	0.55
1:H:368:TYR:N	1:H:369:GLU:CB	2.70	0.55
1:C:111:ARG:HD3	2:C:791:HOH:O	2.06	0.55
1:H:140:TYR:H	1:H:144:GLN:HE21	1.51	0.55
1:C:258:LEU:HD11	1:C:275:ILE:CG2	2.36	0.55
1:A:448:LEU:HD13	1:A:494:ILE:HD12	1.89	0.55
1:D:140:TYR:H	1:D:144:GLN:HE21	1.53	0.55
1:G:30:GLY:N	2:G:738:HOH:O	2.39	0.55
1:C:268:PRO:HG3	1:C:273:LEU:HD11	1.88	0.55
1:E:84:ILE:HG12	1:E:91:VAL:HG22	1.89	0.55
1:E:111:ARG:NH2	1:E:117:ASP:OD2	2.39	0.55
1:G:322:ILE:HG13	1:G:392:MET:HG3	1.89	0.55
1:A:445:SER:HB2	1:A:446:PRO:HD3	1.89	0.54
1:G:308:LYS:HA	1:G:311:GLN:HG3	1.88	0.54
1:B:401:ARG:HH22	1:B:407:VAL:H	1.53	0.54
1:E:321:LYS:HD3	1:E:321:LYS:O	2.07	0.54
1:B:324:GLN:HG2	2:B:719:HOH:O	2.08	0.54
1:H:59:GLN:HE22	1:H:529:LEU:H	1.53	0.54
1:A:380:PRO:HG2	1:A:414:TRP:HE3	1.72	0.54
1:B:111:ARG:NH2	1:B:117:ASP:OD2	2.39	0.54
1:C:401:ARG:HH21	1:C:407:VAL:H	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:ASN:HD22	1:G:385:TYR:HB3	1.71	0.54
1:H:70:VAL:HG22	1:H:71:THR:CG2	2.38	0.54
1:E:286:ARG:HG3	1:E:286:ARG:NH1	2.22	0.54
1:A:140:TYR:H	1:A:144:GLN:HE21	1.54	0.54
1:G:467:PHE:CE1	1:G:471:LEU:HD11	2.43	0.54
1:B:379:MET:HE2	1:B:430:LEU:O	2.07	0.54
1:E:346:GLU:H	1:E:491:GLN:HE22	1.55	0.54
1:G:351:MET:HE1	1:G:501:TYR:HE1	1.72	0.54
1:C:413:GLU:HG2	1:C:414:TRP:N	2.23	0.54
1:E:88:GLY:O	1:E:170:ALA:HA	2.08	0.54
1:E:287:GLU:HB2	1:E:521:LEU:HD13	1.90	0.54
1:F:388:ASN:ND2	1:F:391:LYS:HB2	2.23	0.54
1:F:464:ASN:OD1	1:F:466:GLU:HG2	2.08	0.54
1:F:265:THR:O	2:F:725:HOH:O	2.18	0.54
1:H:291:ASN:HD22	1:H:385:TYR:HB3	1.73	0.53
1:B:286:ARG:HD2	2:B:795:HOH:O	2.08	0.53
1:F:233:TRP:CE3	1:F:234:LYS:HB2	2.42	0.53
1:F:322:ILE:HG13	1:F:392:MET:HG3	1.90	0.53
1:A:89:LYS:HD2	1:A:169:ASN:HA	1.90	0.53
1:D:291:ASN:ND2	1:D:506:GLY:H	1.88	0.53
1:G:390:ARG:NH1	1:G:411:GLU:CB	2.71	0.53
1:A:490:ALA:O	1:A:494:ILE:HG12	2.07	0.53
1:C:414:TRP:O	1:C:417:PHE:HB3	2.09	0.53
1:E:123:SER:HA	1:E:126:PHE:CE2	2.43	0.53
1:C:519:ILE:HG23	1:C:519:ILE:O	2.08	0.53
1:D:322:ILE:HD11	1:D:327:TYR:HE2	1.74	0.53
1:E:314:VAL:HG11	1:E:352:PRO:HG2	1.89	0.53
1:E:319:ILE:HA	1:E:322:ILE:HG23	1.90	0.53
1:A:151:LEU:CD1	1:A:167:LEU:HB3	2.39	0.53
1:H:30:GLY:N	2:H:624:HOH:O	2.41	0.53
1:H:260:LYS:HD3	1:H:260:LYS:N	2.23	0.53
1:A:218:TYR:O	1:A:219:ARG:HD3	2.08	0.53
1:D:339:PRO:HA	1:D:505:HIS:CE1	2.44	0.53
1:F:268:PRO:HB3	1:F:272:GLN:HE21	1.55	0.53
1:H:35:ALA:HB3	1:H:246:ILE:HD13	1.90	0.53
1:A:276:LEU:O	1:A:277:ALA:HB3	2.08	0.53
1:G:447:LEU:HD12	1:G:447:LEU:H	1.72	0.53
1:A:484:LYS:HE3	2:A:669:HOH:O	2.08	0.53
1:B:268:PRO:CB	1:B:272:GLN:HE21	2.22	0.53
1:B:319:ILE:HD11	1:B:333:ARG:NE	2.23	0.53
1:B:431:LEU:HD12	1:B:432:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LYS:NZ	1:C:97:LYS:HB3	2.23	0.53
1:C:268:PRO:CB	1:C:272:GLN:HE21	2.13	0.53
1:F:322:ILE:HD11	1:F:392:MET:CE	2.38	0.53
1:G:249:ASN:HD22	1:G:252:THR:H	1.57	0.53
1:G:274:SER:O	1:G:277:ALA:HB2	2.09	0.53
1:G:436:ASP:H	1:G:442:ASN:HD21	1.54	0.53
1:H:111:ARG:NH2	1:H:117:ASP:OD2	2.42	0.53
1:H:319:ILE:HG12	1:H:333:ARG:CZ	2.39	0.53
1:A:286:ARG:H	1:B:357:GLN:NE2	2.01	0.53
1:A:319:ILE:HA	1:A:322:ILE:HG12	1.90	0.53
1:B:306:ASN:HB3	1:B:309:VAL:HG23	1.91	0.53
1:C:268:PRO:CA	1:C:272:GLN:NE2	2.72	0.53
1:E:319:ILE:O	1:E:323:MET:HG2	2.08	0.53
1:C:268:PRO:HD3	1:C:509:PHE:HB2	1.91	0.52
1:F:513:SER:O	1:F:516:VAL:HG22	2.08	0.52
1:H:390:ARG:O	1:H:394:GLU:HG3	2.09	0.52
1:A:97:LYS:HE2	1:A:161:HIS:NE2	2.23	0.52
1:B:319:ILE:HD11	1:B:333:ARG:HD3	1.89	0.52
1:C:253:ARG:HB3	1:C:265:THR:CG2	2.39	0.52
1:D:291:ASN:O	1:D:505:HIS:CD2	2.59	0.52
1:E:38:ASN:ND2	1:E:221:ASP:H	2.05	0.52
1:G:309:VAL:O	1:G:313:LEU:HG	2.09	0.52
1:G:383:ARG:HG2	1:G:385:TYR:CE2	2.44	0.52
1:A:278:GLN:HG3	1:A:280:ASP:OD2	2.08	0.52
1:C:257:ILE:HD11	1:C:265:THR:OG1	2.10	0.52
1:C:379:MET:CE	1:C:386:ASN:CB	2.85	0.52
1:C:473:LYS:HD3	1:C:486:TYR:CZ	2.45	0.52
1:H:319:ILE:HA	1:H:322:ILE:HG23	1.91	0.52
1:C:287:GLU:OE1	1:C:287:GLU:HA	2.09	0.52
1:D:374:MET:CE	1:D:400:LEU:HD13	2.40	0.52
1:G:392:MET:O	1:G:396:MET:HG3	2.10	0.52
1:A:448:LEU:HD13	1:A:494:ILE:CD1	2.39	0.52
1:A:35:ALA:HB1	2:A:638:HOH:O	2.10	0.52
1:A:436:ASP:H	1:A:442:ASN:ND2	2.07	0.52
1:C:56:ILE:HG13	1:C:57:ALA:N	2.25	0.52
1:A:146:VAL:HG13	1:A:148:ILE:CD1	2.39	0.52
1:C:445:SER:HB2	1:C:446:PRO:HD3	1.91	0.52
1:F:304:PHE:HE1	1:F:374:MET:CE	2.22	0.52
1:F:390:ARG:CZ	1:F:411:GLU:OE1	2.58	0.52
1:G:397:GLN:HG3	1:G:407:VAL:HB	1.91	0.52
1:E:436:ASP:H	1:E:442:ASN:ND2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:390:ARG:NH1	1:H:411:GLU:OE1	2.43	0.51
1:E:34:CYS:SG	1:E:253:ARG:HG2	2.50	0.51
1:A:390:ARG:NH1	1:A:411:GLU:OE1	2.41	0.51
1:D:319:ILE:HA	1:D:322:ILE:CG2	2.40	0.51
1:D:467:PHE:HA	1:D:493:MET:HE3	1.92	0.51
1:G:123:SER:HA	1:G:126:PHE:CE2	2.46	0.51
1:A:268:PRO:HG3	1:A:273:LEU:HD21	1.91	0.51
1:C:419:GLN:O	1:C:423:GLU:HG3	2.11	0.51
1:H:322:ILE:HD11	1:H:327:TYR:CE1	2.43	0.51
1:H:448:LEU:HD13	1:H:494:ILE:HD12	1.92	0.51
1:A:258:LEU:HD23	1:A:279:ARG:HE	1.75	0.51
1:A:360:LYS:HZ2	1:A:370:LYS:HG3	1.71	0.51
1:C:223:LEU:C	1:C:223:LEU:HD12	2.30	0.51
1:C:390:ARG:NH1	1:C:411:GLU:CB	2.74	0.51
1:C:414:TRP:CH2	1:C:418:ILE:HD11	2.46	0.51
1:F:38:ASN:HD21	1:F:221:ASP:N	2.08	0.51
1:F:96:ARG:HG2	1:F:99:VAL:HG23	1.93	0.51
1:B:273:LEU:HD13	1:B:284:VAL:CG1	2.41	0.51
1:C:111:ARG:HH22	1:C:117:ASP:CG	2.14	0.51
1:D:346:GLU:H	1:D:491:GLN:HE22	1.57	0.51
1:H:272:GLN:CG	1:C:251:THR:HG21	2.41	0.51
1:B:382:SER:O	1:B:383:ARG:HD3	2.10	0.51
1:C:340:PRO:HA	1:C:345:PHE:CG	2.45	0.51
1:E:265:THR:HG22	1:E:266:ALA:O	2.11	0.51
1:F:237:VAL:HG23	2:F:616:HOH:O	2.11	0.51
1:H:447:LEU:O	1:H:458:ASN:HA	2.10	0.51
1:D:322:ILE:C	1:D:322:ILE:HD13	2.31	0.51
1:E:82:TRP:HA	1:E:92:THR:O	2.10	0.51
1:F:307:LEU:HD13	1:F:310:ARG:HH12	1.76	0.51
1:G:374:MET:HE2	1:G:405:VAL:HG11	1.93	0.51
1:H:419:GLN:HG3	1:H:420:ARG:H	1.72	0.51
1:B:296:ALA:HA	1:B:500:LEU:HA	1.92	0.51
1:D:249:ASN:ND2	1:D:249:ASN:C	2.64	0.51
1:E:148:ILE:HD12	2:E:679:HOH:O	2.09	0.51
1:D:353:ILE:HD13	1:D:354:PHE:N	2.25	0.50
1:F:288:THR:HG22	1:F:507:MET:SD	2.51	0.50
1:F:411:GLU:HA	2:F:661:HOH:O	2.12	0.50
1:H:142:TYR:OH	1:H:436:ASP:HB3	2.11	0.50
1:B:319:ILE:HG12	1:B:333:ARG:CZ	2.42	0.50
1:D:31:LEU:HD23	1:D:32:VAL:N	2.27	0.50
1:G:250:GLY:HA2	1:G:253:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:HIS:CD2	1:C:214:ILE:HG12	2.46	0.50
1:C:295:TRP:CE3	1:C:396:MET:HE2	2.46	0.50
1:D:111:ARG:NH2	1:D:117:ASP:OD2	2.43	0.50
1:D:137:ASP:HA	2:D:703:HOH:O	2.11	0.50
1:E:322:ILE:HD13	1:E:323:MET:N	2.26	0.50
1:H:154:LYS:HD3	2:H:677:HOH:O	2.12	0.50
1:A:140:TYR:H	1:A:144:GLN:NE2	2.10	0.50
1:B:371:GLY:HA2	1:B:404:GLY:O	2.10	0.50
1:B:519:ILE:HD13	1:B:532:ALA:HA	1.93	0.50
1:D:291:ASN:HD21	1:D:506:GLY:N	1.88	0.50
1:E:31:LEU:HD23	1:E:32:VAL:N	2.26	0.50
1:E:266:ALA:O	1:E:267:HIS:C	2.49	0.50
1:F:275:ILE:O	1:F:278:GLN:HG2	2.12	0.50
1:F:413:GLU:OE2	1:F:415:ASN:HB2	2.11	0.50
1:A:287:GLU:O	2:A:695:HOH:O	2.20	0.50
1:B:307:LEU:O	1:B:311:GLN:HG3	2.11	0.50
1:C:223:LEU:HA	1:C:246:ILE:HD12	1.93	0.50
1:C:291:ASN:O	1:C:505:HIS:HD2	1.94	0.50
1:C:519:ILE:HD11	1:C:529:LEU:CD2	2.42	0.50
1:H:56:ILE:HG13	1:H:57:ALA:N	2.26	0.50
1:E:286:ARG:CG	1:E:507:MET:HE1	2.41	0.50
1:F:38:ASN:ND2	1:F:221:ASP:H	2.06	0.50
1:C:319:ILE:HA	1:C:322:ILE:HG23	1.92	0.50
1:H:368:TYR:O	1:H:370:LYS:HA	2.07	0.50
1:A:360:LYS:HZ3	1:A:370:LYS:HG3	1.77	0.50
1:E:368:TYR:H	1:E:369:GLU:CD	2.16	0.50
1:F:315:HIS:CD2	1:F:358:LEU:CD1	2.95	0.50
1:H:379:MET:CE	1:H:386:ASN:HB3	2.42	0.49
1:A:300:GLU:HB2	1:A:461:ASN:ND2	2.27	0.49
1:A:374:MET:O	1:A:407:VAL:HA	2.11	0.49
1:C:143:PHE:HB3	1:C:148:ILE:HG22	1.93	0.49
1:D:259:THR:OG1	1:D:261:GLU:HG3	2.11	0.49
1:F:152:ILE:HD12	1:F:165:PHE:HD2	1.75	0.49
1:F:289:ASN:ND2	1:F:508:ARG:HH11	2.06	0.49
1:A:220:ARG:O	1:A:221:ASP:HB2	2.12	0.49
1:C:368:TYR:C	1:C:370:LYS:HA	2.32	0.49
1:F:353:ILE:HD13	1:F:354:PHE:N	2.26	0.49
1:A:367:GLY:O	1:A:368:TYR:C	2.50	0.49
1:C:295:TRP:CE3	1:C:396:MET:CE	2.96	0.49
1:G:287:GLU:HB2	1:G:521:LEU:HD13	1.95	0.49
1:E:65:ILE:HG13	1:E:179:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LYS:HD2	1:B:169:ASN:HA	1.95	0.49
1:E:500:LEU:C	1:E:500:LEU:HD12	2.31	0.49
1:H:111:ARG:HH22	1:H:117:ASP:CG	2.16	0.49
1:B:268:PRO:CB	1:B:272:GLN:NE2	2.75	0.49
1:C:453:THR:HG22	1:C:454:PHE:CD1	2.48	0.49
1:D:70:VAL:HG22	1:D:71:THR:N	2.28	0.49
1:G:153:ARG:O	1:G:154:LYS:HG2	2.13	0.49
1:G:473:LYS:HB3	1:G:486:TYR:CE2	2.46	0.49
1:H:519:ILE:HD12	1:H:532:ALA:HA	1.94	0.49
1:G:315:HIS:HB2	1:G:359:ALA:HB2	1.94	0.49
1:H:152:ILE:HD11	1:H:174:PHE:CE1	2.45	0.49
1:H:348:GLN:NE2	1:H:492:SER:HA	2.28	0.49
1:E:294:TYR:OH	1:E:459:PRO:HG3	2.11	0.49
1:F:114:ASN:HB2	1:F:160:ASP:O	2.11	0.49
1:D:354:PHE:CE1	1:D:356:PRO:HG3	2.48	0.49
1:C:363:LEU:HB3	1:C:368:TYR:O	2.13	0.49
1:D:266:ALA:O	1:D:267:HIS:C	2.51	0.49
1:D:358:LEU:O	1:D:358:LEU:HD22	2.12	0.49
1:E:111:ARG:HH22	1:E:117:ASP:CG	2.16	0.49
1:H:124:ARG:HD3	1:H:132:TYR:O	2.13	0.48
1:A:319:ILE:CD1	1:A:333:ARG:HG3	2.40	0.48
1:C:416:THR:HG22	1:C:420:ARG:NE	2.28	0.48
1:G:374:MET:HE1	1:G:400:LEU:HD13	1.95	0.48
1:A:254:ILE:CG2	1:A:276:LEU:HD11	2.43	0.48
1:A:363:LEU:HD13	1:A:368:TYR:O	2.13	0.48
1:C:280:ASP:N	1:C:280:ASP:OD1	2.46	0.48
1:D:98:GLY:HA2	1:D:112:GLU:OE1	2.13	0.48
1:F:59:GLN:HE21	1:F:529:LEU:H	1.61	0.48
1:F:375:SER:HB3	1:F:408:ASN:O	2.14	0.48
1:F:433:TRP:CD2	1:F:447:LEU:HD11	2.48	0.48
1:H:225:ARG:CD	1:H:243:VAL:HG22	2.43	0.48
1:A:201:ASN:OD1	1:A:202:LEU:HD13	2.12	0.48
1:A:414:TRP:NE1	1:A:418:ILE:HD11	2.28	0.48
1:B:470:LEU:HD11	1:B:493:MET:CE	2.43	0.48
1:D:158:VAL:HG23	1:D:159:SER:N	2.28	0.48
1:B:289:ASN:HD22	1:B:508:ARG:HH11	1.61	0.48
1:B:304:PHE:CE2	1:B:427:ASP:HB3	2.48	0.48
1:B:360:LYS:O	1:B:364:THR:HG22	2.14	0.48
1:B:519:ILE:HG23	1:B:519:ILE:O	2.12	0.48
1:E:311:GLN:O	1:E:315:HIS:HD2	1.97	0.48
1:H:110:THR:HB	1:H:189:GLU:OE2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:ASN:HD22	1:H:144:GLN:NE2	2.04	0.48
1:B:70:VAL:HG23	1:B:71:THR:HG23	1.95	0.48
1:C:268:PRO:CA	1:C:272:GLN:HE22	2.26	0.48
1:D:374:MET:CE	1:D:405:VAL:HG11	2.44	0.48
1:H:370:LYS:HD3	1:H:370:LYS:N	2.29	0.48
1:H:500:LEU:HD12	1:H:500:LEU:C	2.34	0.48
1:C:436:ASP:H	1:C:442:ASN:HD21	1.62	0.48
1:D:374:MET:HE3	1:D:400:LEU:HD13	1.96	0.48
1:D:508:ARG:HD2	1:D:521:LEU:HD21	1.95	0.48
1:F:267:HIS:HE1	1:F:527:ILE:HD11	1.79	0.48
1:A:363:LEU:O	1:A:367:GLY:O	2.32	0.48
1:D:416:THR:HG22	1:D:420:ARG:HD2	1.96	0.48
1:H:500:LEU:HD12	1:H:500:LEU:O	2.13	0.48
1:F:361:LYS:O	1:F:364:THR:HG22	2.14	0.48
1:F:500:LEU:HD12	1:F:500:LEU:C	2.33	0.48
1:F:519:ILE:HD12	1:F:519:ILE:HA	1.58	0.48
1:G:52:THR:O	1:G:56:ILE:HG12	2.13	0.48
1:G:137:ASP:HB2	1:G:139:ASN:CB	2.43	0.48
1:A:310:ARG:CD	1:A:498:LEU:O	2.59	0.48
1:B:368:TYR:N	2:B:658:HOH:O	2.45	0.48
1:E:384:ILE:HD13	1:E:384:ILE:N	2.28	0.48
1:H:139:ASN:ND2	1:H:144:GLN:NE2	2.61	0.48
1:H:479:ASP:HB3	1:H:482:LEU:CD1	2.44	0.48
1:H:516:VAL:CG2	1:H:519:ILE:HD13	2.44	0.48
1:C:268:PRO:CB	1:C:272:GLN:HE22	2.25	0.48
1:G:252:THR:O	1:G:256:LYS:HG3	2.14	0.48
1:H:287:GLU:O	1:H:508:ARG:HG3	2.14	0.47
1:H:319:ILE:O	1:H:322:ILE:HG23	2.14	0.47
1:B:97:LYS:HE3	1:B:161:HIS:CE1	2.49	0.47
1:B:470:LEU:HD11	1:B:493:MET:HE1	1.96	0.47
1:D:380:PRO:HA	1:D:411:GLU:OE2	2.14	0.47
1:E:157:ARG:NH2	1:E:160:ASP:OD1	2.47	0.47
1:G:510:GLN:HB2	2:G:748:HOH:O	2.13	0.47
1:G:519:ILE:HG23	1:G:519:ILE:O	2.14	0.47
1:B:374:MET:CE	1:B:405:VAL:HG11	2.44	0.47
1:C:390:ARG:NH1	1:C:411:GLU:HB2	2.29	0.47
1:G:34:CYS:O	1:G:253:ARG:HD3	2.14	0.47
1:H:253:ARG:NH2	2:H:824:HOH:O	2.48	0.47
1:H:268:PRO:CG	1:H:273:LEU:HD21	2.41	0.47
1:C:238:ALA:HB1	1:C:533:ARG:HG3	1.95	0.47
1:D:75:LYS:NZ	1:D:75:LYS:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:480:LEU:HA	1:F:483:ARG:HD2	1.96	0.47
1:A:278:GLN:HA	1:A:279:ARG:O	2.14	0.47
1:A:320:GLU:HA	1:B:349:LYS:HE2	1.97	0.47
1:B:445:SER:HB2	1:B:446:PRO:HD3	1.96	0.47
1:C:309:VAL:O	1:C:313:LEU:HG	2.14	0.47
1:D:287:GLU:HB2	1:D:521:LEU:HD13	1.95	0.47
1:E:220:ARG:NH2	2:E:641:HOH:O	2.48	0.47
1:E:484:LYS:O	1:E:488:ASP:CG	2.53	0.47
1:F:372:PHE:CE1	1:F:374:MET:HE2	2.41	0.47
1:F:413:GLU:HG2	1:F:414:TRP:N	2.30	0.47
1:B:340:PRO:HA	1:B:345:PHE:CG	2.49	0.47
1:E:75:LYS:NZ	1:E:75:LYS:HB3	2.29	0.47
1:F:279:ARG:HB3	1:F:281:ASP:OD1	2.15	0.47
1:G:518:GLY:O	1:G:519:ILE:HD12	2.15	0.47
1:H:125:LEU:HD13	1:H:143:PHE:CG	2.50	0.47
1:A:68:ASP:OD1	1:A:70:VAL:HG22	2.13	0.47
1:A:132:TYR:CE1	1:A:191:ALA:HB1	2.50	0.47
1:D:123:SER:HA	1:D:126:PHE:CE2	2.49	0.47
1:D:469:LEU:O	1:D:473:LYS:HG3	2.14	0.47
1:E:319:ILE:HG12	1:E:333:ARG:NE	2.29	0.47
1:E:368:TYR:N	1:E:369:GLU:CB	2.78	0.47
1:F:157:ARG:NH2	1:F:159:SER:HA	2.30	0.47
1:F:322:ILE:CG1	1:F:392:MET:HG3	2.45	0.47
1:G:291:ASN:O	1:G:505:HIS:CD2	2.63	0.47
1:E:357:GLN:HE21	1:E:357:GLN:HB2	1.58	0.47
1:E:384:ILE:HG22	1:E:506:GLY:HA3	1.97	0.47
1:A:70:VAL:HG23	1:A:71:THR:HG23	1.97	0.47
1:A:223:LEU:C	1:A:223:LEU:HD12	2.36	0.47
1:A:370:LYS:H	1:A:370:LYS:HD3	1.79	0.47
1:B:135:VAL:HA	1:B:136:GLY:HA2	1.50	0.47
1:B:390:ARG:NH1	1:B:411:GLU:HB2	2.30	0.47
1:C:71:THR:O	1:C:72:ALA:HB3	2.15	0.47
1:D:269:SER:HB2	1:D:330:ASN:HD21	1.79	0.47
1:D:500:LEU:HD12	1:D:500:LEU:O	2.15	0.47
1:E:462:TRP:CG	1:E:499:PRO:HB3	2.50	0.47
1:G:158:VAL:HG21	1:G:162:GLN:OE1	2.15	0.47
1:B:124:ARG:HD3	1:B:132:TYR:O	2.14	0.47
1:B:148:ILE:CD1	1:B:177:ASN:HB3	2.45	0.47
1:B:390:ARG:HH12	1:B:411:GLU:HB2	1.80	0.47
1:F:102:HIS:CD2	1:F:214:ILE:HG12	2.50	0.47
1:G:374:MET:O	1:G:407:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:291:ASN:HD21	1:H:506:GLY:H	1.63	0.46
1:A:294:TYR:HA	1:A:503:ILE:HG12	1.97	0.46
1:A:370:LYS:HD3	1:A:370:LYS:N	2.29	0.46
1:B:257:ILE:HG22	1:B:282:ILE:HD12	1.97	0.46
1:D:158:VAL:HG21	1:D:162:GLN:HG2	1.96	0.46
1:E:85:SER:HB3	1:E:90:SER:HB2	1.97	0.46
1:F:73:GLU:HB2	2:F:701:HOH:O	2.15	0.46
1:D:358:LEU:O	1:D:362:LEU:HG	2.15	0.46
1:E:81:ASP:OD2	1:E:83:LYS:HE3	2.14	0.46
1:E:269:SER:O	1:E:273:LEU:HG	2.14	0.46
1:F:269:SER:HB2	1:F:330:ASN:HD21	1.81	0.46
1:F:367:GLY:C	1:F:369:GLU:HB2	2.35	0.46
1:F:416:THR:CG2	1:F:420:ARG:NE	2.78	0.46
1:C:232:TYR:CE2	1:C:234:LYS:HB3	2.50	0.46
1:C:519:ILE:HD13	1:C:532:ALA:HB2	1.97	0.46
1:F:519:ILE:HG23	1:F:519:ILE:O	2.16	0.46
1:G:370:LYS:H	1:G:370:LYS:CD	2.19	0.46
1:A:102:HIS:CD2	1:A:214:ILE:HG12	2.51	0.46
1:B:97:LYS:HB3	1:B:97:LYS:HE2	1.68	0.46
1:D:134:PHE:HB2	2:D:639:HOH:O	2.15	0.46
1:D:355:ASP:OD2	1:D:358:LEU:HB2	2.15	0.46
1:F:111:ARG:NH2	1:F:117:ASP:OD2	2.47	0.46
1:F:322:ILE:HD12	1:F:392:MET:HE2	1.96	0.46
1:G:438:PRO:HD3	1:G:524:PHE:CE2	2.50	0.46
1:B:56:ILE:HG13	1:B:57:ALA:N	2.31	0.46
1:B:132:TYR:HA	1:B:135:VAL:HG13	1.96	0.46
1:A:68:ASP:HB2	1:A:75:LYS:HG2	1.97	0.46
1:A:304:PHE:HE1	1:A:374:MET:CE	2.28	0.46
1:C:216:LYS:HD2	1:C:227:TYR:CE2	2.50	0.46
1:D:101:PHE:O	1:D:109:PRO:HG3	2.16	0.46
1:E:291:ASN:ND2	1:E:506:GLY:H	2.09	0.46
1:F:348:GLN:O	1:F:351:MET:HG2	2.15	0.46
1:F:433:TRP:CG	1:F:447:LEU:HD11	2.50	0.46
1:G:360:LYS:NZ	1:G:370:LYS:CB	2.70	0.46
1:H:367:GLY:C	1:H:369:GLU:HB2	2.35	0.46
1:A:508:ARG:HG2	1:A:521:LEU:HD11	1.98	0.46
1:B:370:LYS:H	1:B:370:LYS:CD	2.28	0.46
1:C:268:PRO:HA	1:C:272:GLN:HE22	1.80	0.46
1:C:519:ILE:CD1	1:C:532:ALA:HB2	2.46	0.46
1:H:272:GLN:HG2	1:C:251:THR:HG21	1.98	0.46
1:A:276:LEU:HD12	1:A:276:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:GLU:H	1:B:491:GLN:NE2	2.02	0.46
1:C:369:GLU:N	1:C:370:LYS:CA	2.71	0.46
1:E:346:GLU:N	1:E:491:GLN:HE22	2.14	0.46
1:H:379:MET:HE2	1:H:431:LEU:HA	1.98	0.46
1:A:288:THR:HG23	1:A:341:THR:HG23	1.98	0.46
1:B:414:TRP:O	1:B:417:PHE:HB3	2.15	0.46
1:C:135:VAL:HA	1:C:136:GLY:HA2	1.58	0.46
1:E:482:LEU:O	1:E:485:GLN:HB3	2.15	0.46
1:C:126:PHE:CD1	1:C:126:PHE:C	2.89	0.45
1:D:380:PRO:HG2	1:D:414:TRP:HE3	1.80	0.45
1:F:152:ILE:HD11	1:F:174:PHE:HE1	1.81	0.45
1:A:319:ILE:HD12	1:A:323:MET:HG2	1.97	0.45
1:C:413:GLU:HG2	1:C:414:TRP:H	1.81	0.45
1:D:135:VAL:HA	1:D:136:GLY:HA2	1.62	0.45
1:E:268:PRO:CD	1:E:509:PHE:HB2	2.44	0.45
1:G:98:GLY:HA2	1:G:112:GLU:OE1	2.16	0.45
1:G:111:ARG:HH22	1:G:117:ASP:CG	2.18	0.45
1:G:377:TRP:HB3	1:G:417:PHE:HE1	1.81	0.45
1:H:238:ALA:HB1	1:H:533:ARG:HG3	1.97	0.45
1:D:319:ILE:O	1:D:322:ILE:HG23	2.17	0.45
1:E:191:ALA:HB2	1:E:203:PHE:CE1	2.51	0.45
1:F:385:TYR:CD1	1:F:432:GLY:HA3	2.51	0.45
1:H:318:ASP:O	1:H:322:ILE:HG22	2.17	0.45
1:A:232:TYR:CE2	1:A:234:LYS:HB3	2.51	0.45
1:D:310:ARG:HD3	1:D:498:LEU:O	2.17	0.45
1:G:238:ALA:CB	1:G:533:ARG:HG3	2.46	0.45
1:G:413:GLU:CD	1:G:415:ASN:H	2.19	0.45
1:A:245:ASP:C	1:A:245:ASP:OD1	2.55	0.45
1:B:269:SER:O	1:B:273:LEU:HG	2.17	0.45
1:B:529:LEU:HG	2:B:806:HOH:O	2.15	0.45
1:D:369:GLU:HB3	1:D:371:GLY:N	2.31	0.45
1:H:367:GLY:HA2	1:H:369:GLU:OE1	2.16	0.45
1:A:123:SER:HA	1:A:126:PHE:CE1	2.51	0.45
1:C:358:LEU:HD22	1:C:362:LEU:HD12	1.97	0.45
1:C:360:LYS:HZ2	1:C:370:LYS:HB2	1.81	0.45
1:E:155:ILE:HD13	1:E:165:PHE:CE2	2.51	0.45
1:E:220:ARG:CD	1:E:220:ARG:N	2.78	0.45
1:H:416:THR:HA	1:H:419:GLN:HG2	1.97	0.45
1:B:374:MET:HE3	1:B:405:VAL:HG11	1.99	0.45
1:C:401:ARG:HH22	1:C:407:VAL:H	1.59	0.45
1:D:111:ARG:HH22	1:D:117:ASP:CG	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:LEU:O	1:E:316:ALA:HB3	2.16	0.45
1:F:254:ILE:HD13	1:F:254:ILE:HA	1.82	0.45
1:F:286:ARG:HB2	1:F:509:PHE:CD1	2.52	0.45
1:F:372:PHE:CE1	1:F:374:MET:CE	2.95	0.45
1:F:467:PHE:HA	1:F:493:MET:HE1	1.98	0.45
1:B:218:TYR:O	1:B:219:ARG:HD3	2.17	0.45
1:B:348:GLN:NE2	1:B:492:SER:HA	2.31	0.45
1:E:215:TYR:CD1	1:E:215:TYR:C	2.89	0.45
1:A:319:ILE:O	1:A:323:MET:HG2	2.16	0.45
1:B:38:ASN:HD21	1:B:221:ASP:H	1.64	0.45
1:B:360:LYS:HZ2	1:B:370:LYS:HG3	1.81	0.45
1:B:403:ILE:HG22	1:B:405:VAL:HG23	1.98	0.45
1:D:516:VAL:HG22	1:D:519:ILE:HD13	1.99	0.45
1:E:445:SER:HB2	1:E:446:PRO:HD3	1.99	0.45
1:F:276:LEU:HB3	1:F:282:ILE:HG21	1.99	0.45
1:B:283:ASN:ND2	1:B:514:ALA:HA	2.32	0.45
1:B:417:PHE:CD2	1:B:418:ILE:HD13	2.52	0.45
1:D:431:LEU:CG	1:D:432:GLY:H	2.27	0.45
1:G:473:LYS:O	1:G:477:THR:HG22	2.17	0.45
1:A:224:VAL:HG13	1:A:244:TYR:HB2	1.99	0.44
1:A:228:LYS:HE2	1:A:237:VAL:HB	1.98	0.44
1:A:368:TYR:HA	2:A:752:HOH:O	2.16	0.44
1:B:367:GLY:O	1:B:368:TYR:C	2.55	0.44
1:B:501:TYR:HA	1:B:502:PRO:HD3	1.86	0.44
1:C:390:ARG:NH1	1:C:411:GLU:HB3	2.32	0.44
1:F:135:VAL:HA	1:F:136:GLY:HA2	1.56	0.44
1:F:269:SER:CB	1:F:330:ASN:HD21	2.29	0.44
1:F:319:ILE:O	1:F:323:MET:HG2	2.17	0.44
1:G:340:PRO:HA	1:G:345:PHE:CG	2.52	0.44
1:C:268:PRO:HB2	1:C:269:SER:H	1.46	0.44
1:D:340:PRO:HA	1:D:345:PHE:CG	2.52	0.44
1:E:363:LEU:HD23	1:E:363:LEU:HA	1.76	0.44
1:G:401:ARG:C	1:G:403:ILE:H	2.21	0.44
1:H:519:ILE:HG23	1:H:519:ILE:O	2.18	0.44
1:A:436:ASP:H	1:A:442:ASN:HD21	1.64	0.44
1:B:275:ILE:HD12	1:B:275:ILE:N	2.29	0.44
1:B:378:ALA:HB3	1:B:411:GLU:HG2	2.00	0.44
1:C:31:LEU:HD23	1:C:31:LEU:C	2.38	0.44
1:E:388:ASN:ND2	1:E:391:LYS:HB2	2.33	0.44
1:H:131:PRO:HB3	1:H:195:LYS:NZ	2.32	0.44
1:H:135:VAL:HA	1:H:136:GLY:HA2	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:517:GLU:HG3	2:H:699:HOH:O	2.16	0.44
1:B:291:ASN:O	1:B:505:HIS:CD2	2.65	0.44
1:D:84:ILE:HG22	1:D:88:GLY:HA2	1.99	0.44
1:F:223:LEU:HD12	1:F:223:LEU:C	2.37	0.44
1:H:266:ALA:O	1:H:267:HIS:O	2.36	0.44
1:B:367:GLY:O	1:B:369:GLU:N	2.51	0.44
1:C:283:ASN:ND2	1:C:514:ALA:HA	2.32	0.44
1:D:148:ILE:HD12	2:D:715:HOH:O	2.18	0.44
1:E:223:LEU:C	1:E:223:LEU:HD12	2.38	0.44
1:F:322:ILE:HD11	1:F:392:MET:HE2	1.99	0.44
1:G:89:LYS:HD3	1:G:169:ASN:HA	1.99	0.44
1:G:294:TYR:CE2	1:G:432:GLY:HA2	2.53	0.44
1:H:33:TYR:HE1	1:H:266:ALA:HB2	1.83	0.44
1:A:135:VAL:HA	1:A:136:GLY:HA2	1.61	0.44
1:C:286:ARG:NH2	1:E:283:ASN:OD1	2.51	0.44
1:C:286:ARG:HB2	1:C:507:MET:HE3	1.98	0.44
1:D:322:ILE:HG13	1:D:392:MET:HG3	1.99	0.44
1:E:228:LYS:HB2	1:E:239:LEU:O	2.17	0.44
1:A:361:LYS:O	1:A:365:GLU:HG3	2.17	0.44
1:C:61:TYR:HB3	1:C:184:VAL:HB	1.98	0.44
1:C:206:TYR:CE1	1:D:199:GLN:HG2	2.52	0.44
1:C:326:VAL:O	1:C:387:PRO:HG2	2.18	0.44
1:G:414:TRP:NE1	1:G:418:ILE:HG13	2.33	0.44
1:H:367:GLY:C	1:H:368:TYR:CD1	2.91	0.44
1:A:31:LEU:C	1:A:31:LEU:HD23	2.38	0.44
1:C:62:ASP:HB2	1:C:78:LEU:HD11	2.00	0.44
1:E:383:ARG:HA	1:E:383:ARG:HD3	1.83	0.44
1:F:322:ILE:HD11	1:F:392:MET:HG3	2.00	0.44
1:G:343:TRP:HZ3	1:G:484:LYS:HG3	1.82	0.44
1:A:228:LYS:CE	1:A:237:VAL:O	2.63	0.44
1:B:288:THR:HB	1:B:507:MET:HG2	1.99	0.44
1:B:306:ASN:HB3	1:B:309:VAL:CG2	2.48	0.44
1:B:319:ILE:HD11	1:B:333:ARG:HD2	1.97	0.44
1:C:142:TYR:OH	1:C:180:THR:HG21	2.18	0.44
1:C:146:VAL:O	1:C:146:VAL:HG22	2.18	0.44
1:C:319:ILE:HD12	1:C:503:ILE:HG23	2.00	0.44
1:C:348:GLN:HG3	1:C:495:ILE:HG13	2.00	0.44
1:D:374:MET:HE2	1:D:405:VAL:HG11	1.99	0.44
1:C:376:ILE:HG13	1:C:407:VAL:HG13	1.99	0.43
1:E:322:ILE:O	1:E:326:VAL:HB	2.18	0.43
1:E:469:LEU:HD12	1:E:469:LEU:HA	1.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:356:PRO:O	1:G:403:ILE:HD11	2.18	0.43
1:G:390:ARG:O	1:G:394:GLU:HG3	2.18	0.43
1:B:85:SER:HB3	1:B:90:SER:HB2	1.99	0.43
1:B:480:LEU:H	1:B:480:LEU:HG	1.67	0.43
1:D:249:ASN:ND2	1:D:252:THR:N	2.50	0.43
1:G:274:SER:O	1:G:277:ALA:CB	2.66	0.43
1:A:291:ASN:O	1:A:505:HIS:CD2	2.70	0.43
1:B:155:ILE:HG22	1:B:163:VAL:HG22	2.01	0.43
1:C:390:ARG:HH12	1:C:411:GLU:HB3	1.84	0.43
1:C:505:HIS:HE1	2:C:610:HOH:O	2.00	0.43
1:D:67:ILE:HD11	1:D:74:PHE:HE1	1.83	0.43
1:D:321:LYS:HA	1:D:321:LYS:CE	2.48	0.43
1:E:273:LEU:HD11	1:E:509:PHE:HB3	2.00	0.43
1:E:403:ILE:HA	1:E:403:ILE:HD12	1.76	0.43
1:H:385:TYR:CD1	1:H:432:GLY:HA3	2.53	0.43
1:B:259:THR:O	1:B:260:LYS:HB2	2.17	0.43
1:D:158:VAL:HG23	1:D:162:GLN:HB3	2.00	0.43
1:E:339:PRO:HB3	1:E:505:HIS:CD2	2.54	0.43
1:A:88:GLY:O	1:A:170:ALA:HA	2.18	0.43
1:C:477:THR:OG1	1:C:478:THR:N	2.52	0.43
1:D:304:PHE:HZ	1:D:374:MET:HB3	1.84	0.43
1:E:374:MET:CE	1:E:405:VAL:HG11	2.48	0.43
1:F:153:ARG:HG3	1:F:168:PHE:CZ	2.52	0.43
1:F:358:LEU:O	1:F:358:LEU:HD22	2.18	0.43
1:G:286:ARG:HB3	1:G:509:PHE:CD2	2.54	0.43
1:G:447:LEU:HD12	1:G:447:LEU:N	2.34	0.43
1:H:381:VAL:HG22	1:H:414:TRP:CE3	2.54	0.43
1:B:346:GLU:HA	1:B:347:PRO:HD3	1.80	0.43
1:C:296:ALA:HA	1:C:500:LEU:HA	1.99	0.43
1:E:269:SER:H	1:E:272:GLN:NE2	2.17	0.43
1:G:61:TYR:HB3	1:G:184:VAL:HB	2.01	0.43
1:G:81:ASP:OD2	1:G:83:LYS:HE3	2.19	0.43
1:G:114:ASN:OD1	1:G:116:ASP:HB2	2.17	0.43
1:H:291:ASN:O	1:H:505:HIS:CD2	2.55	0.43
1:B:286:ARG:HB3	1:B:509:PHE:CD1	2.54	0.43
1:B:289:ASN:ND2	1:B:508:ARG:HH11	2.17	0.43
1:C:351:MET:SD	1:C:495:ILE:HD12	2.58	0.43
1:E:97:LYS:HB3	1:E:97:LYS:HE2	1.37	0.43
1:H:259:THR:OG1	1:H:261:GLU:HB2	2.18	0.43
1:H:445:SER:HB2	1:H:446:PRO:HD3	1.99	0.43
1:A:500:LEU:HD12	1:A:500:LEU:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:MET:CA	2:A:695:HOH:O	2.57	0.43
1:B:363:LEU:HD23	1:B:363:LEU:HA	1.81	0.43
1:C:82:TRP:HA	1:C:92:THR:O	2.18	0.43
1:C:397:GLN:HG3	1:C:407:VAL:HB	2.01	0.43
1:B:123:SER:HA	1:B:126:PHE:CE2	2.54	0.43
1:B:438:PRO:HD3	1:B:524:PHE:CE2	2.54	0.43
1:C:360:LYS:NZ	1:C:370:LYS:HB2	2.34	0.43
1:D:237:VAL:HG23	2:D:722:HOH:O	2.18	0.43
1:D:445:SER:HB2	1:D:446:PRO:HD3	2.01	0.43
1:D:466:GLU:H	1:D:466:GLU:HG2	1.49	0.43
1:G:319:ILE:HA	1:G:322:ILE:CG2	2.49	0.43
1:H:266:ALA:C	1:H:267:HIS:O	2.57	0.43
1:H:300:GLU:HB2	1:H:461:ASN:ND2	2.34	0.43
1:A:158:VAL:HG21	1:A:162:GLN:HG2	2.01	0.43
1:B:111:ARG:HH22	1:B:117:ASP:CG	2.21	0.43
1:D:228:LYS:HG3	1:D:237:VAL:HB	2.01	0.43
1:E:286:ARG:HG3	1:E:507:MET:HE1	2.00	0.43
1:F:380:PRO:HA	1:F:411:GLU:OE2	2.19	0.43
1:G:82:TRP:C	1:G:83:LYS:HG3	2.40	0.43
1:B:308:LYS:HD2	2:B:798:HOH:O	2.18	0.42
1:D:322:ILE:HD11	1:D:327:TYR:CE2	2.53	0.42
1:D:448:LEU:HA	1:D:458:ASN:ND2	2.34	0.42
1:E:77:GLU:O	1:E:233:TRP:CH2	2.72	0.42
1:E:380:PRO:HA	1:E:411:GLU:OE2	2.18	0.42
1:E:414:TRP:CZ2	1:E:418:ILE:HD11	2.54	0.42
1:E:473:LYS:O	1:E:474:ALA:C	2.58	0.42
1:F:358:LEU:C	1:F:358:LEU:HD13	2.38	0.42
1:G:320:GLU:OE1	1:G:320:GLU:HA	2.19	0.42
1:A:199:GLN:HB3	1:A:202:LEU:HD22	2.00	0.42
1:C:481:ASN:H	1:C:481:ASN:HD22	1.66	0.42
1:D:480:LEU:HD23	1:D:480:LEU:HA	1.77	0.42
1:E:295:TRP:CZ3	1:E:317:ILE:CD1	2.91	0.42
1:G:307:LEU:O	1:G:311:GLN:CG	2.67	0.42
1:A:319:ILE:HG12	1:A:333:ARG:CZ	2.49	0.42
1:B:534:LYS:HD2	2:B:761:HOH:O	2.19	0.42
1:C:124:ARG:HD2	1:C:140:TYR:CE1	2.54	0.42
1:C:295:TRP:CZ3	1:C:396:MET:HE2	2.53	0.42
1:C:379:MET:HE3	1:C:386:ASN:HB3	1.93	0.42
1:F:345:PHE:CE2	1:F:347:PRO:HG3	2.54	0.42
1:B:349:LYS:HE3	1:B:349:LYS:HB3	1.83	0.42
1:B:400:LEU:HB3	1:B:405:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:LEU:HD11	1:C:493:MET:CE	2.49	0.42
1:E:84:ILE:CG2	1:E:88:GLY:HA2	2.49	0.42
1:F:317:ILE:HD12	1:F:396:MET:HG2	2.00	0.42
1:G:38:ASN:HB3	1:G:218:TYR:OH	2.20	0.42
1:H:216:LYS:HB3	1:H:225:ARG:O	2.19	0.42
1:A:269:SER:H	1:A:272:GLN:NE2	2.18	0.42
1:C:403:ILE:HA	1:C:403:ILE:HD12	1.82	0.42
1:E:114:ASN:HB2	1:E:160:ASP:O	2.19	0.42
1:G:482:LEU:HD22	1:G:482:LEU:HA	1.84	0.42
1:A:380:PRO:CG	1:A:414:TRP:HE3	2.31	0.42
1:C:140:TYR:H	1:C:144:GLN:NE2	2.18	0.42
1:C:480:LEU:HA	1:C:483:ARG:HB2	2.01	0.42
1:D:279:ARG:NH1	1:D:283:ASN:OD1	2.47	0.42
1:E:348:GLN:NE2	1:E:492:SER:HA	2.34	0.42
1:E:513:SER:O	1:E:516:VAL:HG13	2.19	0.42
1:F:470:LEU:HD11	1:F:493:MET:HE2	2.02	0.42
1:G:59:GLN:HE21	1:G:529:LEU:H	1.68	0.42
1:A:313:LEU:HD13	1:A:374:MET:HE1	2.01	0.42
1:A:346:GLU:H	1:A:491:GLN:HE22	1.68	0.42
1:A:379:MET:HE3	1:A:386:ASN:HB3	1.95	0.42
1:B:142:TYR:OH	1:B:180:THR:HG21	2.20	0.42
1:C:77:GLU:OE1	1:C:234:LYS:HE2	2.19	0.42
1:C:206:TYR:OH	1:D:201:ASN:OD1	2.34	0.42
1:D:67:ILE:HD11	1:D:74:PHE:CE1	2.55	0.42
1:E:508:ARG:NH2	1:E:525:GLY:O	2.30	0.42
1:F:431:LEU:HG	1:F:432:GLY:H	1.85	0.42
1:G:124:ARG:HD3	1:G:140:TYR:OH	2.20	0.42
1:G:374:MET:HE3	1:G:405:VAL:HG11	2.00	0.42
1:B:258:LEU:CD2	1:B:279:ARG:NH1	2.82	0.42
1:C:448:LEU:HD13	1:C:494:ILE:HD12	2.02	0.42
1:D:381:VAL:HG21	1:D:383:ARG:HH21	1.84	0.42
1:D:416:THR:O	1:D:419:GLN:HB3	2.20	0.42
1:E:234:LYS:HD2	1:E:235:HIS:CD2	2.55	0.42
1:F:104:THR:HG22	1:F:214:ILE:CG2	2.49	0.42
1:G:417:PHE:O	1:G:421:ILE:HG12	2.20	0.42
1:H:448:LEU:CD1	1:H:494:ILE:HD12	2.50	0.42
1:B:327:TYR:O	1:B:328:TYR:C	2.57	0.42
1:C:215:TYR:HA	1:C:226:PHE:CD1	2.54	0.42
1:A:368:TYR:H	1:A:369:GLU:HB2	1.76	0.42
1:A:417:PHE:O	1:A:421:ILE:HG12	2.20	0.42
1:B:413:GLU:OE2	1:B:415:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASN:HD22	1:C:385:TYR:HB3	1.85	0.42
1:C:519:ILE:HD11	1:C:529:LEU:HD22	2.01	0.42
1:D:268:PRO:HB3	1:D:272:GLN:HE21	1.85	0.42
1:G:368:TYR:CD1	1:G:368:TYR:N	2.87	0.42
1:H:115:ALA:HB1	1:H:163:VAL:HG23	2.02	0.41
1:A:151:LEU:HD12	1:A:151:LEU:O	2.20	0.41
1:A:383:ARG:HA	1:A:383:ARG:HD3	1.85	0.41
1:G:110:THR:HG22	1:G:189:GLU:CD	2.40	0.41
1:H:223:LEU:HD12	1:H:223:LEU:O	2.20	0.41
1:A:253:ARG:HB3	1:A:265:THR:CG2	2.40	0.41
1:C:258:LEU:HD11	1:C:275:ILE:HG21	2.01	0.41
1:C:332:LEU:O	1:C:504:ALA:HB1	2.21	0.41
1:E:64:LEU:HD23	1:E:64:LEU:HA	1.88	0.41
1:E:454:PHE:CG	1:E:454:PHE:O	2.70	0.41
1:G:34:CYS:HB3	1:G:253:ARG:CG	2.42	0.41
1:H:31:LEU:HD23	1:H:32:VAL:N	2.35	0.41
1:H:475:LEU:HD23	1:H:475:LEU:HA	1.93	0.41
1:D:108:THR:HA	1:D:109:PRO:HD2	1.89	0.41
1:D:132:TYR:O	1:D:135:VAL:HG13	2.21	0.41
1:E:132:TYR:O	1:E:135:VAL:HG13	2.19	0.41
1:F:82:TRP:HA	1:F:92:THR:O	2.20	0.41
1:H:377:TRP:CE2	1:H:426:HIS:HB3	2.55	0.41
1:A:97:LYS:HB3	1:A:97:LYS:NZ	2.35	0.41
1:A:142:TYR:OH	1:A:436:ASP:HB3	2.21	0.41
1:B:374:MET:CE	1:B:400:LEU:HD13	2.49	0.41
1:C:137:ASP:O	1:C:138:ALA:HB3	2.19	0.41
1:E:302:PRO:HA	1:E:305:ASP:OD1	2.20	0.41
1:E:319:ILE:O	1:E:319:ILE:HG13	2.15	0.41
1:F:390:ARG:NH2	1:F:411:GLU:HB3	2.35	0.41
1:G:381:VAL:HG22	1:G:414:TRP:CE3	2.55	0.41
1:H:294:TYR:CE2	1:H:432:GLY:HA2	2.55	0.41
1:H:321:LYS:O	1:H:321:LYS:HD3	2.20	0.41
1:A:380:PRO:HD2	1:A:414:TRP:CE3	2.55	0.41
1:A:508:ARG:HD3	1:A:521:LEU:HD22	2.03	0.41
1:C:123:SER:HA	1:C:126:PHE:CE2	2.55	0.41
1:C:403:ILE:O	1:C:403:ILE:HG23	2.20	0.41
1:E:101:PHE:HE2	1:E:117:ASP:OD2	2.04	0.41
1:F:315:HIS:CD2	1:F:358:LEU:HD11	2.56	0.41
1:A:31:LEU:HD23	1:A:32:VAL:N	2.36	0.41
1:A:276:LEU:H	1:A:276:LEU:CD1	2.33	0.41
1:A:287:GLU:HG3	1:A:521:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ARG:NH1	1:C:497:GLN:O	2.54	0.41
1:D:97:LYS:HE3	1:D:161:HIS:CD2	2.55	0.41
1:D:379:MET:HA	1:D:380:PRO:HD2	1.91	0.41
1:G:225:ARG:HD3	1:G:241:GLN:OE1	2.21	0.41
1:H:448:LEU:HD13	1:H:494:ILE:CD1	2.51	0.41
1:A:413:GLU:OE2	1:A:415:ASN:HB2	2.20	0.41
1:B:319:ILE:HA	1:B:322:ILE:HD12	2.03	0.41
1:C:319:ILE:HG12	1:C:333:ARG:CZ	2.50	0.41
1:D:360:LYS:CE	1:D:370:LYS:HE3	2.50	0.41
1:E:151:LEU:HG	1:E:167:LEU:HD22	2.02	0.41
1:E:218:TYR:O	1:E:219:ARG:HD3	2.20	0.41
1:E:310:ARG:HD3	1:E:498:LEU:O	2.21	0.41
1:F:436:ASP:H	1:F:442:ASN:ND2	2.19	0.41
1:H:97:LYS:HB3	1:H:97:LYS:HE2	1.70	0.41
1:A:228:LYS:HB2	1:A:240:GLU:HA	2.03	0.41
1:A:314:VAL:HG13	1:A:501:TYR:CD2	2.56	0.41
1:A:327:TYR:CZ	1:A:504:ALA:HB3	2.55	0.41
1:A:362:LEU:HA	1:A:362:LEU:HD23	1.75	0.41
1:B:414:TRP:CE2	1:B:418:ILE:HG13	2.56	0.41
1:B:417:PHE:HD2	1:B:418:ILE:HD13	1.86	0.41
1:C:322:ILE:C	1:C:322:ILE:CD1	2.86	0.41
1:C:353:ILE:HD12	1:C:353:ILE:HA	1.58	0.41
1:C:377:TRP:CE2	1:C:426:HIS:HB3	2.56	0.41
1:D:363:LEU:HD23	1:D:363:LEU:HA	1.86	0.41
1:D:388:ASN:ND2	1:D:391:LYS:HB2	2.36	0.41
1:E:34:CYS:SG	1:E:256:LYS:HD2	2.61	0.41
1:E:215:TYR:HA	1:E:226:PHE:HD1	1.86	0.41
1:E:353:ILE:HD13	1:E:353:ILE:HA	1.92	0.41
1:F:224:VAL:HG13	1:F:244:TYR:HB2	2.02	0.41
1:F:322:ILE:CD1	1:F:392:MET:HG3	2.51	0.41
1:F:343:TRP:CE2	1:F:440:PRO:HG2	2.56	0.41
1:G:487:TYR:O	1:G:491:GLN:HG3	2.21	0.41
1:G:508:ARG:NH2	1:G:525:GLY:O	2.54	0.41
1:A:214:ILE:HD11	1:A:229:ASN:HA	2.03	0.41
1:A:448:LEU:CD1	1:A:494:ILE:HD12	2.51	0.41
1:C:519:ILE:HD11	1:C:529:LEU:HD23	2.03	0.41
1:D:31:LEU:HD23	1:D:31:LEU:C	2.42	0.41
1:D:158:VAL:HG22	1:D:162:GLN:C	2.40	0.41
1:E:467:PHE:CE1	1:E:494:ILE:HD11	2.56	0.41
1:F:418:ILE:HD13	1:F:418:ILE:HA	1.85	0.41
1:G:258:LEU:CD2	1:G:279:ARG:HH12	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:LEU:O	1:G:311:GLN:HG3	2.20	0.41
1:A:508:ARG:HD3	1:A:521:LEU:CD2	2.51	0.40
1:C:273:LEU:O	1:C:274:SER:C	2.59	0.40
1:D:301:ARG:HA	1:D:302:PRO:HD2	1.73	0.40
1:E:137:ASP:C	1:E:139:ASN:N	2.74	0.40
1:F:245:ASP:OD2	1:F:256:LYS:NZ	2.51	0.40
1:G:82:TRP:HA	1:G:92:THR:O	2.21	0.40
1:G:137:ASP:HB2	1:G:139:ASN:HB3	2.03	0.40
1:G:319:ILE:CG2	1:G:333:ARG:CZ	2.98	0.40
1:A:400:LEU:HB3	1:A:405:VAL:HB	2.03	0.40
1:B:35:ALA:HB3	1:B:246:ILE:HD13	2.03	0.40
1:B:291:ASN:ND2	1:B:385:TYR:HB3	2.36	0.40
1:D:362:LEU:HA	1:D:362:LEU:HD23	1.75	0.40
1:F:464:ASN:HA	1:F:465:PRO:HD3	1.84	0.40
1:G:135:VAL:HA	1:G:136:GLY:HA2	1.67	0.40
1:G:266:ALA:O	1:G:267:HIS:C	2.59	0.40
1:G:340:PRO:HA	1:G:345:PHE:CD2	2.57	0.40
1:H:403:ILE:HG22	1:H:405:VAL:HG23	2.04	0.40
1:H:438:PRO:O	1:H:440:PRO:HD3	2.22	0.40
1:H:513:SER:O	1:H:516:VAL:CG1	2.69	0.40
1:A:286:ARG:HB3	1:A:509:PHE:CD1	2.57	0.40
1:A:314:VAL:HG11	1:A:352:PRO:HG2	2.03	0.40
1:A:435:ALA:HB1	1:A:437:THR:O	2.21	0.40
1:B:379:MET:HE2	1:B:379:MET:HB3	1.92	0.40
1:B:436:ASP:H	1:B:442:ASN:HD21	1.68	0.40
1:D:364:THR:C	1:D:366:ALA:H	2.25	0.40
1:D:431:LEU:HG	1:D:432:GLY:N	2.31	0.40
1:D:519:ILE:O	1:D:519:ILE:HG13	2.21	0.40
1:E:68:ASP:HB2	1:E:75:LYS:HG3	2.03	0.40
1:H:225:ARG:HG3	1:H:225:ARG:NH1	2.35	0.40
1:A:272:GLN:OE1	1:D:251:THR:HG21	2.22	0.40
1:B:38:ASN:ND2	1:B:221:ASP:H	2.18	0.40
1:C:467:PHE:CE1	1:C:471:LEU:HD11	2.57	0.40
1:D:373:ASP:OD1	1:D:406:ASN:HB2	2.22	0.40
1:D:470:LEU:HD11	1:D:493:MET:HE2	2.02	0.40
1:G:229:ASN:OD1	1:G:229:ASN:C	2.60	0.40
1:G:259:THR:O	1:G:260:LYS:HB2	2.20	0.40
1:H:275:ILE:O	1:H:275:ILE:HG23	2.22	0.40
1:H:475:LEU:HG	2:H:606:HOH:O	2.20	0.40
1:A:84:ILE:HD12	1:A:84:ILE:N	2.36	0.40
1:B:33:TYR:OH	1:B:266:ALA:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:MET:HE2	1:C:509:PHE:CZ	2.57	0.40
1:D:369:GLU:HB3	1:D:370:LYS:C	2.42	0.40
1:D:438:PRO:HD3	1:D:524:PHE:CE2	2.57	0.40
1:E:135:VAL:HA	1:E:136:GLY:HA2	1.64	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	503/541 (93%)	474 (94%)	25 (5%)	4 (1%)	19	22
1	B	503/541 (93%)	478 (95%)	21 (4%)	4 (1%)	19	22
1	C	503/541 (93%)	470 (93%)	29 (6%)	4 (1%)	19	22
1	D	503/541 (93%)	470 (93%)	30 (6%)	3 (1%)	25	29
1	E	503/541 (93%)	471 (94%)	29 (6%)	3 (1%)	25	29
1	F	503/541 (93%)	473 (94%)	28 (6%)	2 (0%)	34	40
1	G	503/541 (93%)	474 (94%)	24 (5%)	5 (1%)	15	16
1	H	503/541 (93%)	481 (96%)	18 (4%)	4 (1%)	19	22
All	All	4024/4328 (93%)	3791 (94%)	204 (5%)	29 (1%)	22	25

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	266	ALA
1	H	268	PRO
1	A	276	LEU
1	B	267	HIS
1	B	268	PRO
1	B	368	TYR

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Mol	Chain	Res	Type
1	B	369	GLU
1	C	266	ALA
1	C	267	HIS
1	C	268	PRO
1	D	369	GLU
1	F	268	PRO
1	A	279	ARG
1	A	369	GLU
1	C	369	GLU
1	E	267	HIS
1	E	369	GLU
1	G	278	GLN
1	G	369	GLU
1	H	272	GLN
1	E	268	PRO
1	G	336	SER
1	G	368	TYR
1	D	318	ASP
1	H	267	HIS
1	A	267	HIS
1	D	267	HIS
1	G	267	HIS
1	F	275	ILE

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	438/472 (93%)	405 (92%)	33 (8%)	13	16
1	B	438/472 (93%)	404 (92%)	34 (8%)	12	14
1	C	438/472 (93%)	405 (92%)	33 (8%)	13	16
1	D	438/472 (93%)	403 (92%)	35 (8%)	12	14
1	E	438/472 (93%)	397 (91%)	41 (9%)	8	9
1	F	438/472 (93%)	392 (90%)	46 (10%)	7	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	438/472 (93%)	394 (90%)	44 (10%)	7	8
1	H	438/472 (93%)	397 (91%)	41 (9%)	8	9
All	All	3504/3776 (93%)	3197 (91%)	307 (9%)	10	11

All (307) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	34	CYS
1	H	70	VAL
1	H	75	LYS
1	H	76	SER
1	H	81	ASP
1	H	96	ARG
1	H	97	LYS
1	H	110	THR
1	H	111	ARG
1	H	124	ARG
1	H	135	VAL
1	H	146	VAL
1	H	158	VAL
1	H	159	SER
1	H	163	VAL
1	H	217	GLU
1	H	220	ARG
1	H	224	VAL
1	H	260	LYS
1	H	261	GLU
1	H	275	ILE
1	H	278	GLN
1	H	280	ASP
1	H	286	ARG
1	H	319	ILE
1	H	322	ILE
1	H	332	LEU
1	H	358	LEU
1	H	363	LEU
1	H	364	THR
1	H	368	TYR
1	H	369	GLU
1	H	370	LYS
1	H	384	ILE

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Mol	Chain	Res	Type
1	H	482	LEU
1	H	508	ARG
1	H	513	SER
1	H	516	VAL
1	H	519	ILE
1	H	521	LEU
1	H	534	LYS
1	A	76	SER
1	A	110	THR
1	A	111	ARG
1	A	124	ARG
1	A	137	ASP
1	A	157	ARG
1	A	158	VAL
1	A	159	SER
1	A	202	LEU
1	A	216	LYS
1	A	220	ARG
1	A	224	VAL
1	A	251	THR
1	A	269	SER
1	A	287	GLU
1	A	288	THR
1	A	317	ILE
1	A	319	ILE
1	A	321	LYS
1	A	332	LEU
1	A	358	LEU
1	A	363	LEU
1	A	364	THR
1	A	368	TYR
1	A	370	LYS
1	A	375	SER
1	A	408	ASN
1	A	453	THR
1	A	482	LEU
1	A	493	MET
1	A	516	VAL
1	A	521	LEU
1	A	534	LYS
1	B	34	CYS
1	B	75	LYS

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Mol	Chain	Res	Type
1	B	86	LYS
1	B	97	LYS
1	B	110	THR
1	B	111	ARG
1	B	124	ARG
1	B	146	VAL
1	B	148	ILE
1	B	169	ASN
1	B	220	ARG
1	B	224	VAL
1	B	234	LYS
1	B	274	SER
1	B	288	THR
1	B	319	ILE
1	B	321	LYS
1	B	332	LEU
1	B	349	LYS
1	B	358	LEU
1	B	368	TYR
1	B	370	LYS
1	B	379	MET
1	B	383	ARG
1	B	401	ARG
1	B	403	ILE
1	B	411	GLU
1	B	413	GLU
1	B	416	THR
1	B	431	LEU
1	B	485	GLN
1	B	516	VAL
1	B	519	ILE
1	B	521	LEU
1	C	34	CYS
1	C	84	ILE
1	C	110	THR
1	C	111	ARG
1	C	124	ARG
1	C	148	ILE
1	C	158	VAL
1	C	202	LEU
1	C	216	LYS
1	C	220	ARG

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Mol	Chain	Res	Type
1	C	224	VAL
1	C	267	HIS
1	C	269	SER
1	C	280	ASP
1	C	287	GLU
1	C	319	ILE
1	C	321	LYS
1	C	322	ILE
1	C	332	LEU
1	C	353	ILE
1	C	358	LEU
1	C	369	GLU
1	C	383	ARG
1	C	401	ARG
1	C	403	ILE
1	C	413	GLU
1	C	416	THR
1	C	419	GLN
1	C	447	LEU
1	C	453	THR
1	C	496	GLU
1	C	516	VAL
1	C	521	LEU
1	D	34	CYS
1	D	70	VAL
1	D	110	THR
1	D	111	ARG
1	D	124	ARG
1	D	135	VAL
1	D	146	VAL
1	D	148	ILE
1	D	202	LEU
1	D	224	VAL
1	D	249	ASN
1	D	274	SER
1	D	276	LEU
1	D	279	ARG
1	D	280	ASP
1	D	287	GLU
1	D	288	THR
1	D	319	ILE
1	D	321	LYS

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Mol	Chain	Res	Type
1	D	322	ILE
1	D	324	GLN
1	D	332	LEU
1	D	353	ILE
1	D	357	GLN
1	D	358	LEU
1	D	379	MET
1	D	383	ARG
1	D	384	ILE
1	D	390	ARG
1	D	401	ARG
1	D	455	SER
1	D	466	GLU
1	D	477	THR
1	D	516	VAL
1	D	521	LEU
1	E	34	CYS
1	E	65	ILE
1	E	70	VAL
1	E	86	LYS
1	E	90	SER
1	E	96	ARG
1	E	97	LYS
1	E	110	THR
1	E	111	ARG
1	E	124	ARG
1	E	135	VAL
1	E	146	VAL
1	E	158	VAL
1	E	201	ASN
1	E	202	LEU
1	E	216	LYS
1	E	220	ARG
1	E	224	VAL
1	E	225	ARG
1	E	234	LYS
1	E	275	ILE
1	E	278	GLN
1	E	286	ARG
1	E	319	ILE
1	E	321	LYS
1	E	322	ILE

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Mol	Chain	Res	Type
1	E	332	LEU
1	E	357	GLN
1	E	358	LEU
1	E	363	LEU
1	E	403	ILE
1	E	408	ASN
1	E	416	THR
1	E	448	LEU
1	E	451	THR
1	E	477	THR
1	E	480	LEU
1	E	482	LEU
1	E	516	VAL
1	E	520	THR
1	E	521	LEU
1	F	34	CYS
1	F	36	GLU
1	F	70	VAL
1	F	75	LYS
1	F	83	LYS
1	F	86	LYS
1	F	111	ARG
1	F	124	ARG
1	F	135	VAL
1	F	137	ASP
1	F	139	ASN
1	F	146	VAL
1	F	148	ILE
1	F	158	VAL
1	F	163	VAL
1	F	187	SER
1	F	202	LEU
1	F	220	ARG
1	F	224	VAL
1	F	249	ASN
1	F	260	LYS
1	F	265	THR
1	F	269	SER
1	F	274	SER
1	F	280	ASP
1	F	286	ARG
1	F	287	GLU

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Mol	Chain	Res	Type
1	F	319	ILE
1	F	321	LYS
1	F	322	ILE
1	F	332	LEU
1	F	353	ILE
1	F	357	GLN
1	F	364	THR
1	F	368	TYR
1	F	375	SER
1	F	384	ILE
1	F	413	GLU
1	F	453	THR
1	F	466	GLU
1	F	477	THR
1	F	507	MET
1	F	519	ILE
1	F	521	LEU
1	F	533	ARG
1	F	534	LYS
1	G	34	CYS
1	G	75	LYS
1	G	86	LYS
1	G	90	SER
1	G	96	ARG
1	G	111	ARG
1	G	124	ARG
1	G	135	VAL
1	G	137	ASP
1	G	202	LEU
1	G	224	VAL
1	G	241	GLN
1	G	249	ASN
1	G	260	LYS
1	G	265	THR
1	G	275	ILE
1	G	287	GLU
1	G	288	THR
1	G	319	ILE
1	G	321	LYS
1	G	322	ILE
1	G	324	GLN
1	G	332	LEU

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Mol	Chain	Res	Type
1	G	353	ILE
1	G	358	LEU
1	G	368	TYR
1	G	369	GLU
1	G	370	LYS
1	G	384	ILE
1	G	390	ARG
1	G	402	LYS
1	G	403	ILE
1	G	425	ARG
1	G	447	LEU
1	G	454	PHE
1	G	463	CYS
1	G	473	LYS
1	G	477	THR
1	G	482	LEU
1	G	508	ARG
1	G	516	VAL
1	G	519	ILE
1	G	521	LEU
1	G	534	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	38	ASN
1	H	58	ASN
1	H	59	GLN
1	H	139	ASN
1	H	144	GLN
1	H	235	HIS
1	H	249	ASN
1	H	291	ASN
1	H	324	GLN
1	H	330	ASN
1	H	348	GLN
1	H	442	ASN
1	H	491	GLN
1	H	497	GLN
1	H	505	HIS
1	A	38	ASN
1	A	59	GLN

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Mol	Chain	Res	Type
1	A	144	GLN
1	A	162	GLN
1	A	241	GLN
1	A	249	ASN
1	A	291	ASN
1	A	324	GLN
1	A	348	GLN
1	A	442	ASN
1	A	491	GLN
1	A	505	HIS
1	B	38	ASN
1	B	59	GLN
1	B	139	ASN
1	B	144	GLN
1	B	205	GLN
1	B	249	ASN
1	B	272	GLN
1	B	291	ASN
1	B	348	GLN
1	B	357	GLN
1	B	442	ASN
1	B	491	GLN
1	B	505	HIS
1	C	38	ASN
1	C	59	GLN
1	C	139	ASN
1	C	144	GLN
1	C	249	ASN
1	C	272	GLN
1	C	291	ASN
1	C	324	GLN
1	C	330	ASN
1	C	357	GLN
1	C	388	ASN
1	C	419	GLN
1	C	442	ASN
1	C	481	ASN
1	C	491	GLN
1	C	497	GLN
1	C	505	HIS
1	D	38	ASN
1	D	59	GLN

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Mol	Chain	Res	Type
1	D	139	ASN
1	D	144	GLN
1	D	249	ASN
1	D	267	HIS
1	D	278	GLN
1	D	291	ASN
1	D	330	ASN
1	D	348	GLN
1	D	357	GLN
1	D	491	GLN
1	D	505	HIS
1	D	510	GLN
1	E	38	ASN
1	E	59	GLN
1	E	139	ASN
1	E	144	GLN
1	E	150	GLN
1	E	249	ASN
1	E	272	GLN
1	E	278	GLN
1	E	291	ASN
1	E	315	HIS
1	E	324	GLN
1	E	348	GLN
1	E	357	GLN
1	E	419	GLN
1	E	442	ASN
1	E	491	GLN
1	E	505	HIS
1	E	510	GLN
1	F	38	ASN
1	F	59	GLN
1	F	139	ASN
1	F	144	GLN
1	F	205	GLN
1	F	249	ASN
1	F	267	HIS
1	F	272	GLN
1	F	289	ASN
1	F	324	GLN
1	F	330	ASN
1	F	348	GLN

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Mol	Chain	Res	Type
1	F	357	GLN
1	F	408	ASN
1	F	442	ASN
1	F	485	GLN
1	F	491	GLN
1	F	497	GLN
1	F	505	HIS
1	F	510	GLN
1	G	38	ASN
1	G	59	GLN
1	G	139	ASN
1	G	144	GLN
1	G	205	GLN
1	G	249	ASN
1	G	272	GLN
1	G	278	GLN
1	G	291	ASN
1	G	330	ASN
1	G	348	GLN
1	G	442	ASN
1	G	497	GLN
1	G	505	HIS

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 monosaccharides 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	505/541 (93%)	-0.33	3 (0%) 89 91	13, 25, 45, 63	0
1	B	505/541 (93%)	-0.23	6 (1%) 79 82	14, 24, 46, 71	0
1	C	505/541 (93%)	-0.26	4 (0%) 86 89	14, 25, 45, 66	0
1	D	505/541 (93%)	-0.25	8 (1%) 72 77	15, 27, 51, 72	0
1	E	505/541 (93%)	-0.11	9 (1%) 68 74	17, 31, 59, 78	0
1	F	505/541 (93%)	-0.20	4 (0%) 86 89	18, 30, 53, 72	0
1	G	505/541 (93%)	-0.18	13 (2%) 56 62	17, 30, 56, 82	0
1	H	505/541 (93%)	-0.40	1 (0%) 95 96	13, 22, 41, 55	0
All	All	4040/4328 (93%)	-0.24	48 (1%) 79 82	13, 27, 51, 82	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	266	ALA	5.9
1	G	275	ILE	5.5
1	G	369	GLU	5.2
1	C	369	GLU	4.9
1	H	369	GLU	3.8
1	F	70	VAL	3.7
1	G	454	PHE	3.6
1	B	278	GLN	3.5
1	F	369	GLU	3.5
1	B	369	GLU	3.5
1	E	482	LEU	3.2
1	E	454	PHE	3.1
1	G	278	GLN	3.0
1	E	369	GLU	3.0
1	D	267	HIS	2.9
1	C	267	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	367	GLY	2.8
1	G	370	LYS	2.8
1	G	478	THR	2.6
1	D	480	LEU	2.6
1	B	266	ALA	2.6
1	E	269	SER	2.6
1	E	357	GLN	2.5
1	B	86	LYS	2.5
1	B	480	LEU	2.5
1	F	367	GLY	2.5
1	D	482	LEU	2.5
1	G	274	SER	2.4
1	D	370	LYS	2.4
1	E	403	ILE	2.4
1	G	476	ASP	2.4
1	C	266	ALA	2.4
1	E	272	GLN	2.2
1	A	273	LEU	2.2
1	E	480	LEU	2.2
1	D	369	GLU	2.2
1	G	480	LEU	2.2
1	A	86	LYS	2.2
1	G	479	ASP	2.2
1	D	401	ARG	2.2
1	G	271	ALA	2.1
1	G	401	ARG	2.1
1	E	273	LEU	2.1
1	C	227	TYR	2.1
1	B	275	ILE	2.0
1	G	267	HIS	2.0
1	A	136	GLY	2.0
1	D	404	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.