



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:45 PM GMT

PDB ID : 3LML
Title : Crystal Structure of the sheath tail protein Lin1278 from *Listeria innocua*, Northeast Structural Genomics Consortium Target LkR115
Authors : Forouhar, F.; Neely, H.; Seetharaman, J.; Mao, M.; Xiao, R.; Patel, D.J.; Ciccosanti, C.; Wang, H.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2010-01-31
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

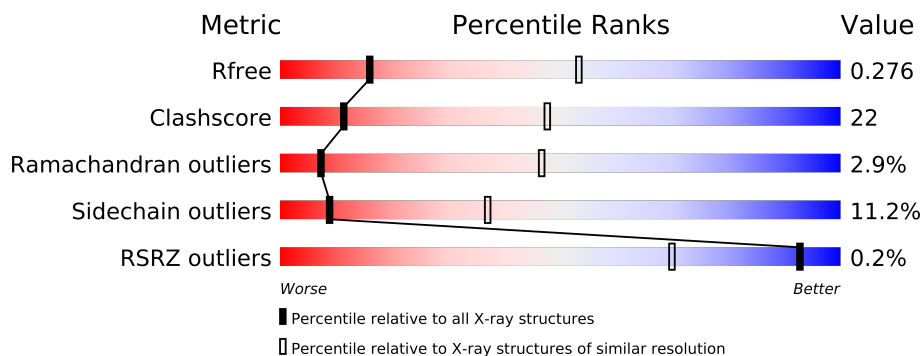
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	460	
1	B	460	
1	C	460	
1	D	460	
1	E	460	
1	F	460	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20036 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Lin1278 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	Se	0	0	0
			3376	2117	565	690	4			
1	B	435	Total	C	N	O	Se	0	0	0
			3338	2093	558	683	4			
1	C	438	Total	C	N	O	Se	0	0	0
			3359	2106	561	688	4			
1	D	434	Total	C	N	O	Se	0	0	0
			3326	2084	557	681	4			
1	E	431	Total	C	N	O	Se	0	0	0
			3302	2068	553	677	4			
1	F	435	Total	C	N	O	Se	0	0	0
			3335	2089	558	684	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	453	LEU	-	EXPRESSION TAG	UNP Q92CB1
A	454	GLU	-	EXPRESSION TAG	UNP Q92CB1
A	455	HIS	-	EXPRESSION TAG	UNP Q92CB1
A	456	HIS	-	EXPRESSION TAG	UNP Q92CB1
A	457	HIS	-	EXPRESSION TAG	UNP Q92CB1
A	458	HIS	-	EXPRESSION TAG	UNP Q92CB1
A	459	HIS	-	EXPRESSION TAG	UNP Q92CB1
A	460	HIS	-	EXPRESSION TAG	UNP Q92CB1
B	453	LEU	-	EXPRESSION TAG	UNP Q92CB1
B	454	GLU	-	EXPRESSION TAG	UNP Q92CB1
B	455	HIS	-	EXPRESSION TAG	UNP Q92CB1
B	456	HIS	-	EXPRESSION TAG	UNP Q92CB1
B	457	HIS	-	EXPRESSION TAG	UNP Q92CB1
B	458	HIS	-	EXPRESSION TAG	UNP Q92CB1
B	459	HIS	-	EXPRESSION TAG	UNP Q92CB1
B	460	HIS	-	EXPRESSION TAG	UNP Q92CB1
C	453	LEU	-	EXPRESSION TAG	UNP Q92CB1

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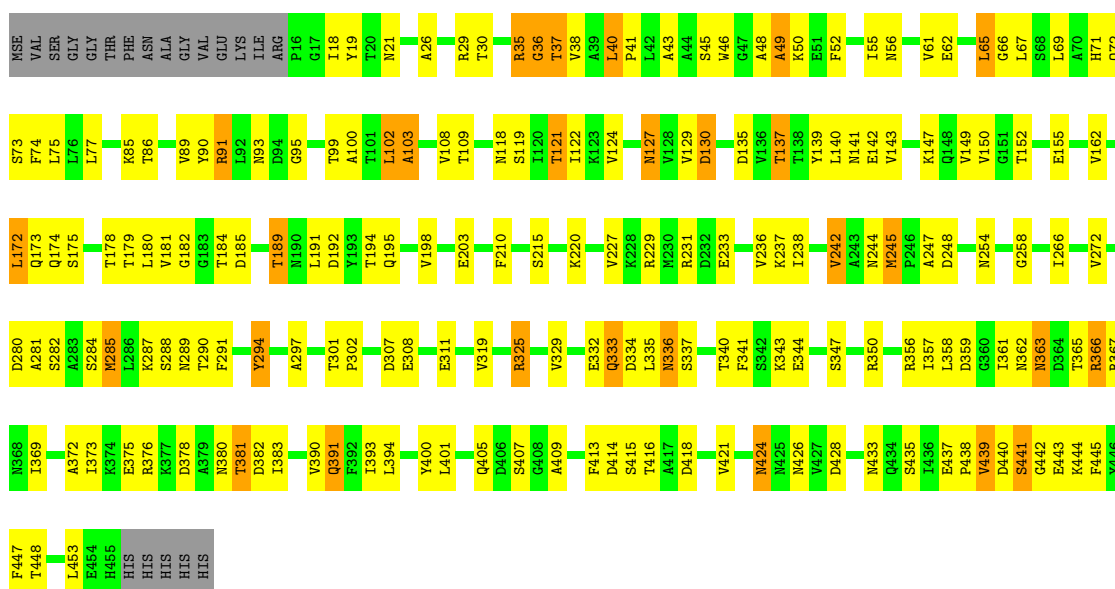
Chain	Residue	Modelled	Actual	Comment	Reference
C	454	GLU	-	EXPRESSION TAG	UNP Q92CB1
C	455	HIS	-	EXPRESSION TAG	UNP Q92CB1
C	456	HIS	-	EXPRESSION TAG	UNP Q92CB1
C	457	HIS	-	EXPRESSION TAG	UNP Q92CB1
C	458	HIS	-	EXPRESSION TAG	UNP Q92CB1
C	459	HIS	-	EXPRESSION TAG	UNP Q92CB1
C	460	HIS	-	EXPRESSION TAG	UNP Q92CB1
D	453	LEU	-	EXPRESSION TAG	UNP Q92CB1
D	454	GLU	-	EXPRESSION TAG	UNP Q92CB1
D	455	HIS	-	EXPRESSION TAG	UNP Q92CB1
D	456	HIS	-	EXPRESSION TAG	UNP Q92CB1
D	457	HIS	-	EXPRESSION TAG	UNP Q92CB1
D	458	HIS	-	EXPRESSION TAG	UNP Q92CB1
D	459	HIS	-	EXPRESSION TAG	UNP Q92CB1
D	460	HIS	-	EXPRESSION TAG	UNP Q92CB1
E	453	LEU	-	EXPRESSION TAG	UNP Q92CB1
E	454	GLU	-	EXPRESSION TAG	UNP Q92CB1
E	455	HIS	-	EXPRESSION TAG	UNP Q92CB1
E	456	HIS	-	EXPRESSION TAG	UNP Q92CB1
E	457	HIS	-	EXPRESSION TAG	UNP Q92CB1
E	458	HIS	-	EXPRESSION TAG	UNP Q92CB1
E	459	HIS	-	EXPRESSION TAG	UNP Q92CB1
E	460	HIS	-	EXPRESSION TAG	UNP Q92CB1
F	453	LEU	-	EXPRESSION TAG	UNP Q92CB1
F	454	GLU	-	EXPRESSION TAG	UNP Q92CB1
F	455	HIS	-	EXPRESSION TAG	UNP Q92CB1
F	456	HIS	-	EXPRESSION TAG	UNP Q92CB1
F	457	HIS	-	EXPRESSION TAG	UNP Q92CB1
F	458	HIS	-	EXPRESSION TAG	UNP Q92CB1
F	459	HIS	-	EXPRESSION TAG	UNP Q92CB1
F	460	HIS	-	EXPRESSION TAG	UNP Q92CB1

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 errors 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.

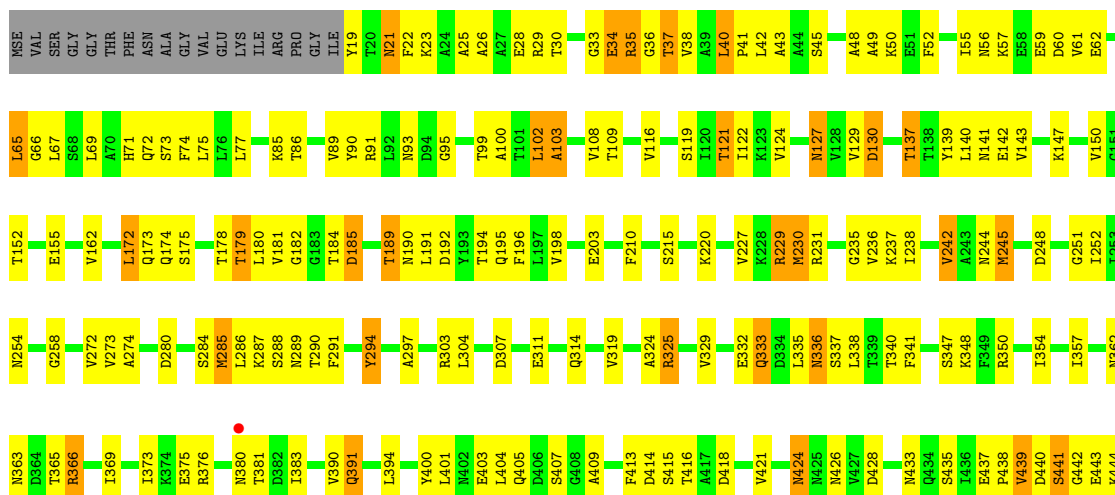
• Molecule 1: Lin1278 protein

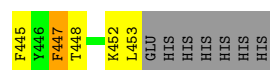
Chain A:



• Molecule 1: Lin1278 protein

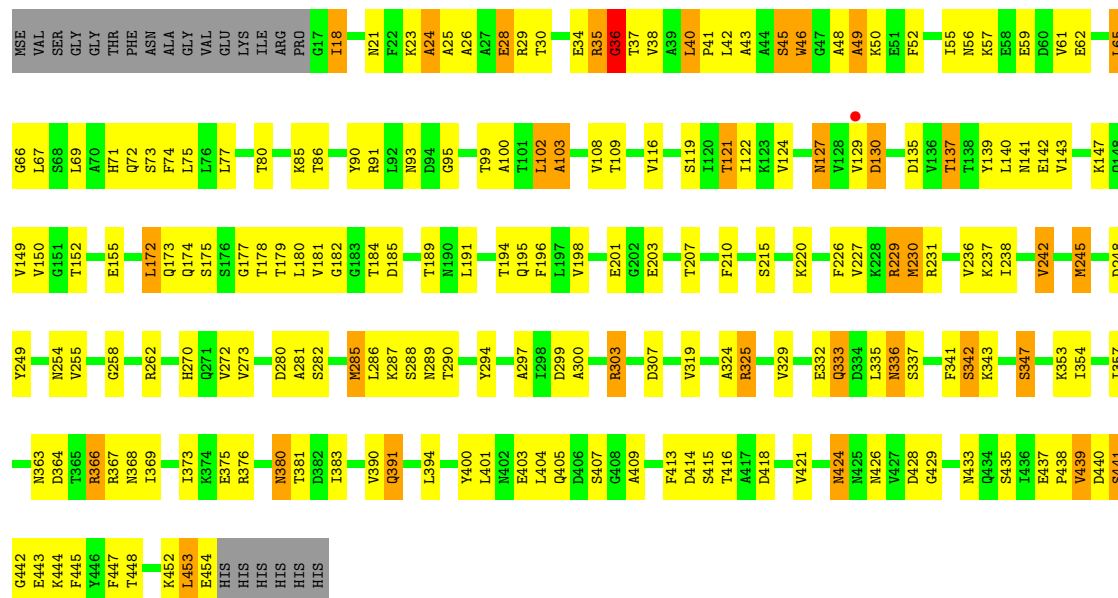
Chain B:





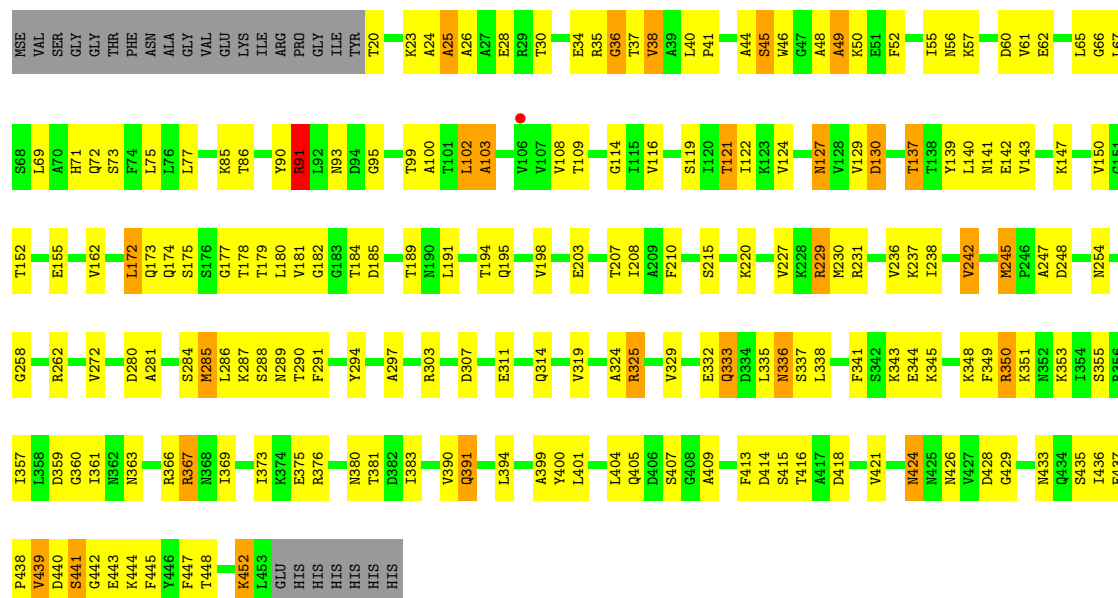
• Molecule 1: Lin1278 protein

Chain C:



• Molecule 1: Lin1278 protein

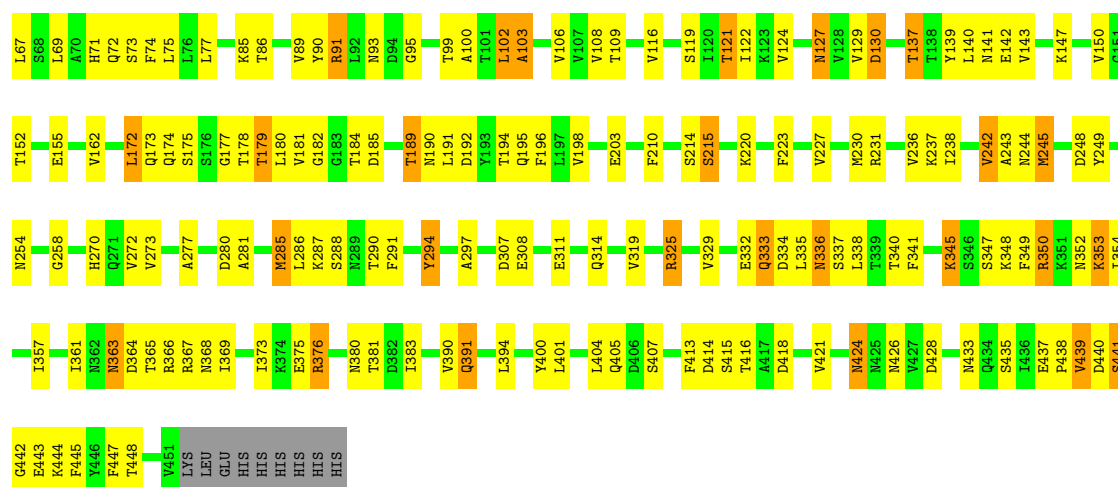
Chain D:



• Molecule 1: Lin1278 protein

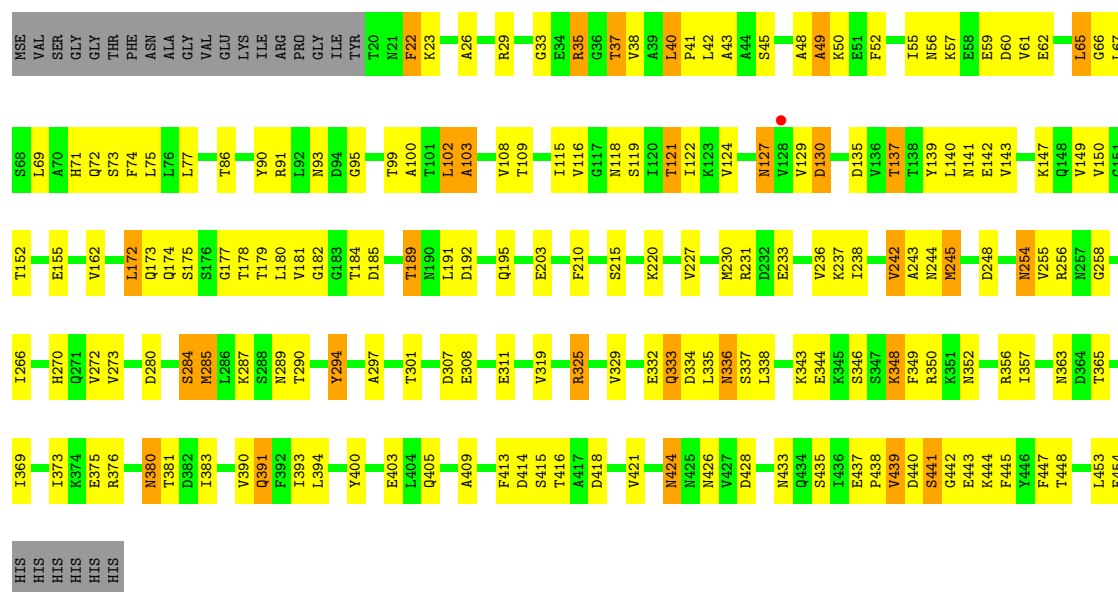
Chain E:





• Molecule 1: Lin1278 protein

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.31Å 153.72Å 217.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 3.30 29.86 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.3 (19.96-3.30) 97.6 (29.86-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.49 (at 3.31Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.230 , 0.260 0.249 , 0.276	Depositor DCC
R_{free} test set	2248 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 4.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 88641 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	20036	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.51	0/3418	0.68	3/4627 (0.1%)
1	B	0.47	0/3378	0.65	3/4573 (0.1%)
1	C	0.52	1/3399 (0.0%)	0.99	11/4601 (0.2%)
1	D	0.49	0/3365	1.01	11/4555 (0.2%)
1	E	0.49	0/3341	0.65	3/4523 (0.1%)
1	F	0.49	1/3374 (0.0%)	0.66	2/4567 (0.0%)
All	All	0.49	2/20275 (0.0%)	0.79	33/27446 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	290	THR	CA-CB	-5.82	1.38	1.53
1	F	290	THR	CA-CB	-5.22	1.39	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	91	ARG	NE-CZ-NH2	-23.73	108.43	120.30
1	D	91	ARG	NE-CZ-NH1	22.72	131.66	120.30
1	C	229	ARG	NE-CZ-NH2	-22.48	109.06	120.30
1	D	262	ARG	NE-CZ-NH2	-21.40	109.60	120.30
1	C	229	ARG	NE-CZ-NH1	20.89	130.74	120.30
1	C	303	ARG	NE-CZ-NH1	-20.69	109.96	120.30
1	C	303	ARG	NE-CZ-NH2	20.12	130.36	120.30
1	D	262	ARG	NE-CZ-NH1	19.62	130.11	120.30
1	D	325	ARG	NE-CZ-NH2	-19.18	110.71	120.30
1	C	325	ARG	NE-CZ-NH2	-18.39	111.11	120.30
1	D	325	ARG	NE-CZ-NH1	17.25	128.92	120.30
1	C	325	ARG	NE-CZ-NH1	16.95	128.78	120.30
1	C	229	ARG	CD-NE-CZ	10.65	138.52	123.60
1	E	325	ARG	NE-CZ-NH1	-10.21	115.20	120.30
1	D	91	ARG	CD-NE-CZ	9.91	137.48	123.60
1	A	325	ARG	NE-CZ-NH1	-9.80	115.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	262	ARG	CD-NE-CZ	9.74	137.24	123.60
1	C	303	ARG	CD-NE-CZ	9.31	136.63	123.60
1	B	325	ARG	NE-CZ-NH1	-9.13	115.73	120.30
1	F	325	ARG	NE-CZ-NH2	8.85	124.72	120.30
1	C	325	ARG	CD-NE-CZ	8.73	135.82	123.60
1	D	325	ARG	CD-NE-CZ	8.67	135.74	123.60
1	F	325	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	E	325	ARG	NE-CZ-NH2	8.45	124.52	120.30
1	A	325	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	B	325	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	D	229	ARG	NE-CZ-NH1	-6.41	117.09	120.30
1	C	36	GLY	N-CA-C	6.15	128.47	113.10
1	B	229	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	A	91	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	D	303	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	E	91	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	C	262	ARG	NE-CZ-NH1	-5.08	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3376	0	3356	152	0
1	B	3338	0	3321	158	0
1	C	3359	0	3341	162	0
1	D	3326	0	3312	146	0
1	E	3302	0	3281	160	0
1	F	3335	0	3318	141	0
All	All	20036	0	19929	889	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (889) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:35:ARG:HH12	1:B:284:SER:HA	0.95	1.11
1:A:285:MSE:HG2	1:A:357:ILE:HD13	1.17	1.10
1:B:35:ARG:NH1	1:B:284:SER:HA	1.75	1.01
1:C:285:MSE:HE3	1:C:357:ILE:HG23	1.45	0.98
1:A:233:GLU:HB2	1:C:229:ARG:HD3	1.45	0.94
1:A:285:MSE:HE3	1:A:357:ILE:HG23	1.46	0.94
1:B:285:MSE:HG2	1:B:357:ILE:HG12	1.52	0.91
1:E:55:ILE:HD11	1:E:77:LEU:HD11	1.52	0.91
1:D:30:THR:HG21	1:D:407:SER:HB2	1.53	0.91
1:B:55:ILE:HD11	1:B:77:LEU:HD11	1.51	0.90
1:B:285:MSE:HE3	1:B:357:ILE:HG23	1.54	0.89
1:D:285:MSE:HG2	1:D:357:ILE:HG13	1.55	0.88
1:D:55:ILE:HD11	1:D:77:LEU:HD11	1.56	0.88
1:B:35:ARG:HH12	1:B:284:SER:CA	1.84	0.88
1:A:37:THR:HB	1:A:86:THR:HB	1.54	0.88
1:E:366:ARG:HB2	1:E:366:ARG:HH21	1.38	0.87
1:E:215:SER:HB3	1:F:301:THR:HB	1.57	0.87
1:C:55:ILE:HD11	1:C:77:LEU:HD11	1.55	0.86
1:E:345:LYS:HD2	1:E:345:LYS:O	1.76	0.86
1:E:30:THR:HG21	1:E:407:SER:HB2	1.58	0.85
1:D:229:ARG:HD2	1:F:233:GLU:HB2	1.57	0.85
1:E:30:THR:HG23	1:E:286:LEU:HD11	1.58	0.85
1:F:99:THR:HG22	1:F:100:ALA:H	1.41	0.85
1:E:99:THR:HG22	1:E:100:ALA:H	1.42	0.84
1:D:40:LEU:HD12	1:D:41:PRO:HD2	1.59	0.84
1:E:366:ARG:NH2	1:E:366:ARG:HB2	1.93	0.83
1:A:99:THR:HG22	1:A:100:ALA:H	1.41	0.83
1:C:43:ALA:HB1	1:C:93:ASN:HD22	1.42	0.83
1:C:43:ALA:HB1	1:C:93:ASN:ND2	1.94	0.82
1:C:99:THR:HG22	1:C:100:ALA:H	1.45	0.82
1:F:285:MSE:HG2	1:F:357:ILE:HG12	1.60	0.82
1:A:35:ARG:O	1:A:85:LYS:HB3	1.78	0.82
1:D:44:ALA:HB3	1:D:91:ARG:HG3	1.61	0.81
1:C:366:ARG:HB2	1:C:366:ARG:HH21	1.44	0.81
1:A:55:ILE:HD11	1:A:77:LEU:HD11	1.63	0.81
1:B:428:ASP:O	1:B:453:LEU:HG	1.81	0.81
1:D:237:LYS:H	1:D:363:ASN:HD21	1.26	0.81
1:B:99:THR:HG22	1:B:100:ALA:H	1.45	0.81
1:B:319:VAL:HG23	1:B:332:GLU:HB2	1.64	0.80
1:F:55:ILE:HD11	1:F:77:LEU:HD11	1.62	0.80
1:D:285:MSE:HE2	1:D:409:ALA:HB1	1.64	0.80
1:B:102:LEU:HD11	1:B:122:ILE:HG21	1.64	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:179:THR:CG2	1:F:181:VAL:HG23	2.11	0.80
1:E:102:LEU:HD11	1:E:122:ILE:HG21	1.64	0.80
1:A:365:THR:O	1:A:369:ILE:HG12	1.82	0.80
1:E:350:ARG:HB2	1:E:350:ARG:HH21	1.47	0.80
1:A:319:VAL:HG23	1:A:332:GLU:HB2	1.63	0.79
1:D:99:THR:HG22	1:D:100:ALA:H	1.47	0.79
1:F:285:MSE:HE3	1:F:357:ILE:HG23	1.64	0.79
1:E:405:GLN:HE22	1:E:413:PHE:H	1.31	0.79
1:E:341:PHE:HA	1:E:345:LYS:HE2	1.64	0.78
1:C:30:THR:HB	1:C:286:LEU:HD11	1.63	0.78
1:F:137:THR:HG22	1:F:147:LYS:HG3	1.65	0.78
1:C:319:VAL:HG23	1:C:332:GLU:HB2	1.66	0.78
1:F:40:LEU:HD23	1:F:41:PRO:HD2	1.66	0.77
1:E:319:VAL:HG23	1:E:332:GLU:HB2	1.64	0.77
1:A:248:ASP:OD1	1:A:340:THR:HG22	1.83	0.77
1:C:405:GLN:HE22	1:C:413:PHE:H	1.32	0.77
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.47	0.77
1:F:102:LEU:HD11	1:F:122:ILE:HG21	1.67	0.77
1:F:37:THR:HB	1:F:86:THR:HB	1.67	0.77
1:C:285:MSE:HG2	1:C:357:ILE:HG12	1.66	0.77
1:D:319:VAL:HG23	1:D:332:GLU:HB2	1.67	0.77
1:D:102:LEU:HD11	1:D:122:ILE:HG21	1.65	0.76
1:F:285:MSE:HE2	1:F:409:ALA:HB1	1.67	0.76
1:D:338:LEU:HG	1:D:341:PHE:HE1	1.51	0.76
1:E:99:THR:HG23	1:E:109:THR:HG22	1.67	0.75
1:A:366:ARG:HB2	1:A:366:ARG:CZ	2.15	0.75
1:F:319:VAL:HG23	1:F:332:GLU:HB2	1.69	0.74
1:B:43:ALA:HB1	1:B:93:ASN:HD22	1.53	0.74
1:C:102:LEU:HD11	1:C:122:ILE:HG21	1.68	0.74
1:A:102:LEU:HD11	1:A:122:ILE:HG21	1.68	0.74
1:D:405:GLN:HE22	1:D:413:PHE:H	1.34	0.73
1:A:229:ARG:HG2	1:C:229:ARG:NH2	2.04	0.73
1:D:99:THR:HG23	1:D:109:THR:HG22	1.69	0.73
1:F:405:GLN:HE22	1:F:413:PHE:H	1.36	0.73
1:A:137:THR:HG22	1:A:147:LYS:HG3	1.70	0.73
1:A:248:ASP:CG	1:A:340:THR:HG22	2.09	0.72
1:A:99:THR:HG23	1:A:109:THR:HG22	1.69	0.72
1:A:118:ASN:HB3	1:B:179:THR:HG23	1.72	0.72
1:E:248:ASP:OD1	1:E:340:THR:HG22	1.89	0.72
1:E:27:ALA:O	1:E:31:LYS:HB2	1.89	0.72
1:B:140:LEU:O	1:B:141:ASN:HB2	1.90	0.72
1:E:373:ILE:HD13	1:E:383:ILE:HD12	1.70	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:137:THR:HG22	1:E:147:LYS:HG3	1.72	0.72
1:B:103:ALA:HB1	1:B:173:GLN:HB2	1.72	0.72
1:F:140:LEU:O	1:F:141:ASN:HB2	1.89	0.71
1:A:35:ARG:O	1:A:85:LYS:CB	2.38	0.71
1:C:119:SER:HB3	1:C:141:ASN:ND2	2.05	0.71
1:B:405:GLN:HE22	1:B:413:PHE:H	1.34	0.71
1:F:356:ARG:HG2	1:F:356:ARG:HH11	1.55	0.71
1:F:99:THR:HG23	1:F:109:THR:HG22	1.71	0.71
1:D:137:THR:HG22	1:D:147:LYS:HG3	1.73	0.71
1:D:429:GLY:HA3	1:D:452:LYS:HA	1.70	0.71
1:D:45:SER:O	1:D:114:GLY:HA3	1.91	0.71
1:D:140:LEU:O	1:D:141:ASN:HB2	1.90	0.71
1:C:103:ALA:HB1	1:C:173:GLN:HB2	1.72	0.70
1:A:373:ILE:HD13	1:A:383:ILE:HD12	1.73	0.70
1:D:103:ALA:HB1	1:D:173:GLN:HB2	1.73	0.70
1:E:103:ALA:HB1	1:E:173:GLN:HB2	1.73	0.70
1:D:338:LEU:HG	1:D:341:PHE:CE1	2.25	0.70
1:A:405:GLN:HE22	1:A:413:PHE:H	1.40	0.70
1:A:40:LEU:HD23	1:A:41:PRO:HD2	1.73	0.70
1:A:119:SER:HB3	1:A:141:ASN:ND2	2.06	0.70
1:A:229:ARG:HG2	1:C:229:ARG:CZ	2.22	0.70
1:C:140:LEU:O	1:C:141:ASN:HB2	1.92	0.70
1:F:119:SER:HB3	1:F:141:ASN:ND2	2.06	0.70
1:A:266:ILE:HD11	1:B:190:ASN:H	1.55	0.69
1:E:119:SER:HB3	1:E:141:ASN:ND2	2.07	0.69
1:E:21:ASN:HD22	1:E:22:PHE:N	1.90	0.69
1:E:179:THR:HG22	1:F:181:VAL:HG23	1.74	0.69
1:A:356:ARG:HH11	1:A:356:ARG:CG	2.03	0.69
1:D:119:SER:HB3	1:D:141:ASN:ND2	2.07	0.69
1:A:140:LEU:O	1:A:141:ASN:HB2	1.93	0.69
1:E:439:VAL:HG23	1:E:440:ASP:H	1.57	0.69
1:C:99:THR:HG23	1:C:109:THR:HG22	1.74	0.69
1:C:366:ARG:NH2	1:C:366:ARG:HB2	2.07	0.69
1:A:439:VAL:HG23	1:A:440:ASP:H	1.58	0.69
1:C:137:THR:HG22	1:C:147:LYS:HG3	1.75	0.69
1:B:439:VAL:HG23	1:B:440:ASP:H	1.58	0.69
1:A:248:ASP:OD2	1:A:340:THR:HG22	1.93	0.68
1:A:103:ALA:HB1	1:A:173:GLN:HB2	1.73	0.68
1:F:352:ASN:O	1:F:356:ARG:HG3	1.94	0.68
1:B:137:THR:HG22	1:B:147:LYS:HG3	1.76	0.68
1:F:103:ALA:HB1	1:F:173:GLN:H	1.59	0.68
1:B:405:GLN:NE2	1:B:413:PHE:H	1.92	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:237:LYS:HB2	1:E:363:ASN:HD21	1.58	0.68
1:F:103:ALA:HB1	1:F:173:GLN:HB2	1.74	0.68
1:F:37:THR:HA	1:F:86:THR:O	1.93	0.68
1:B:414:ASP:OD2	1:B:416:THR:HB	1.94	0.68
1:C:373:ILE:HD13	1:C:383:ILE:HD12	1.76	0.67
1:D:405:GLN:NE2	1:D:413:PHE:H	1.91	0.67
1:E:140:LEU:O	1:E:141:ASN:HB2	1.93	0.67
1:B:43:ALA:HB1	1:B:93:ASN:ND2	2.09	0.67
1:B:119:SER:HB3	1:B:141:ASN:ND2	2.09	0.67
1:B:99:THR:HG23	1:B:109:THR:HG22	1.75	0.67
1:C:369:ILE:O	1:C:373:ILE:HG12	1.95	0.67
1:D:37:THR:HG22	1:D:86:THR:HB	1.77	0.67
1:C:29:ARG:HA	1:C:35:ARG:NH2	2.10	0.67
1:C:121:THR:HG23	1:C:139:TYR:HB2	1.77	0.66
1:E:365:THR:O	1:E:369:ILE:HD13	1.94	0.66
1:F:373:ILE:HD13	1:F:383:ILE:HD12	1.76	0.66
1:C:285:MSE:HE1	1:C:404:LEU:HD13	1.77	0.66
1:E:405:GLN:NE2	1:E:413:PHE:H	1.92	0.66
1:A:336:ASN:HD21	1:A:350:ARG:HA	1.60	0.66
1:F:150:VAL:HB	1:F:155:GLU:HB2	1.78	0.66
1:C:405:GLN:NE2	1:C:413:PHE:H	1.93	0.66
1:B:40:LEU:HD13	1:B:42:LEU:HD11	1.78	0.66
1:E:285:MSE:HE3	1:E:357:ILE:HG22	1.77	0.65
1:E:103:ALA:HB1	1:E:173:GLN:H	1.58	0.65
1:F:405:GLN:NE2	1:F:413:PHE:H	1.94	0.65
1:A:103:ALA:HB1	1:A:173:GLN:H	1.62	0.65
1:E:285:MSE:HE3	1:E:357:ILE:CG2	2.27	0.65
1:C:439:VAL:HG23	1:C:440:ASP:H	1.61	0.65
1:E:190:ASN:ND2	1:F:266:ILE:HD11	2.11	0.65
1:B:248:ASP:OD1	1:B:340:THR:HG22	1.96	0.65
1:F:99:THR:HG22	1:F:100:ALA:N	2.10	0.65
1:A:99:THR:HG22	1:A:100:ALA:N	2.11	0.65
1:D:439:VAL:HG23	1:D:440:ASP:H	1.61	0.65
1:E:99:THR:HG22	1:E:100:ALA:N	2.11	0.65
1:B:103:ALA:HB1	1:B:173:GLN:H	1.62	0.65
1:A:369:ILE:O	1:A:373:ILE:HG12	1.97	0.64
1:A:18:ILE:HD12	1:A:372:ALA:HA	1.79	0.64
1:F:439:VAL:HG23	1:F:440:ASP:H	1.61	0.64
1:B:373:ILE:HD13	1:B:383:ILE:HD12	1.78	0.64
1:B:365:THR:O	1:B:369:ILE:HG13	1.97	0.64
1:A:150:VAL:HB	1:A:155:GLU:HB2	1.80	0.64
1:A:121:THR:HG23	1:A:139:TYR:HB2	1.80	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:103:ALA:HB1	1:C:173:GLN:H	1.62	0.64
1:B:150:VAL:HB	1:B:155:GLU:HB2	1.79	0.64
1:D:373:ILE:HD13	1:D:383:ILE:HD12	1.80	0.64
1:E:336:ASN:HD21	1:E:350:ARG:HA	1.62	0.64
1:F:414:ASP:OD2	1:F:416:THR:HB	1.98	0.64
1:D:124:VAL:HG21	1:D:172:LEU:HD22	1.79	0.64
1:C:18:ILE:HD12	1:C:18:ILE:H	1.61	0.64
1:E:366:ARG:CB	1:E:366:ARG:HH21	2.11	0.63
1:B:99:THR:HG22	1:B:100:ALA:N	2.12	0.63
1:E:414:ASP:OD2	1:E:416:THR:HB	1.98	0.63
1:D:229:ARG:HD3	1:F:233:GLU:OE2	1.98	0.63
1:D:231:ARG:NH1	1:D:359:ASP:OD2	2.31	0.63
1:A:343:LYS:NZ	1:A:344:GLU:HG3	2.13	0.63
1:F:121:THR:HG23	1:F:139:TYR:HB2	1.81	0.63
1:E:150:VAL:HB	1:E:155:GLU:HB2	1.79	0.63
1:B:124:VAL:HG21	1:B:172:LEU:HD22	1.81	0.63
1:D:353:LYS:O	1:D:357:ILE:HD13	1.98	0.62
1:F:258:GLY:HA2	1:F:272:VAL:HG21	1.81	0.62
1:B:45:SER:OG	1:B:185:ASP:OD2	2.16	0.62
1:C:366:ARG:CB	1:C:366:ARG:HH21	2.12	0.62
1:D:363:ASN:O	1:D:366:ARG:HG2	1.99	0.62
1:D:290:THR:O	1:D:291:PHE:HB2	1.99	0.62
1:C:324:ALA:HB2	1:F:380:ASN:HB2	1.81	0.62
1:C:150:VAL:HB	1:C:155:GLU:HB2	1.81	0.62
1:D:150:VAL:HB	1:D:155:GLU:HB2	1.80	0.62
1:D:103:ALA:HB1	1:D:173:GLN:H	1.63	0.62
1:E:124:VAL:HG21	1:E:172:LEU:HD22	1.81	0.62
1:E:350:ARG:HB2	1:E:350:ARG:NH2	2.15	0.62
1:B:29:ARG:O	1:B:285:MSE:HB2	2.00	0.61
1:C:285:MSE:HE2	1:C:409:ALA:HB1	1.82	0.61
1:A:258:GLY:HA2	1:A:272:VAL:HG21	1.82	0.61
1:D:121:THR:HG23	1:D:139:TYR:HB2	1.81	0.61
1:A:414:ASP:OD2	1:A:416:THR:HB	2.00	0.61
1:C:99:THR:HG22	1:C:100:ALA:N	2.12	0.61
1:F:40:LEU:HD23	1:F:41:PRO:CD	2.29	0.61
1:F:237:LYS:HB2	1:F:363:ASN:ND2	2.16	0.61
1:E:121:THR:HG23	1:E:139:TYR:HB2	1.82	0.61
1:A:405:GLN:NE2	1:A:413:PHE:H	1.98	0.61
1:A:266:ILE:HD11	1:B:190:ASN:N	2.15	0.61
1:C:28:GLU:C	1:C:35:ARG:HH21	2.04	0.61
1:E:45:SER:O	1:E:46:TRP:HB2	2.01	0.61
1:B:285:MSE:HE1	1:B:404:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:426:ASN:HB2	1:D:428:ASP:OD1	2.00	0.61
1:C:414:ASP:OD2	1:C:416:THR:HB	2.00	0.61
1:B:35:ARG:HG3	1:B:36:GLY:N	2.14	0.60
1:F:124:VAL:HG21	1:F:172:LEU:HD22	1.83	0.60
1:A:61:VAL:HG21	1:A:69:LEU:HD13	1.82	0.60
1:B:290:THR:O	1:B:291:PHE:HB2	2.00	0.60
1:B:426:ASN:HB2	1:B:428:ASP:OD1	2.01	0.60
1:D:348:LYS:HD2	1:D:348:LYS:N	2.15	0.60
1:D:99:THR:HG22	1:D:100:ALA:N	2.15	0.60
1:E:41:PRO:HD3	1:E:196:PHE:CZ	2.35	0.60
1:E:43:ALA:HB1	1:E:93:ASN:HD22	1.67	0.60
1:B:30:THR:HG22	1:B:286:LEU:HD21	1.84	0.60
1:B:341:PHE:CE1	1:B:347:SER:HA	2.37	0.60
1:A:285:MSE:HE2	1:A:409:ALA:HB1	1.84	0.60
1:D:343:LYS:HG3	1:D:344:GLU:OE1	2.02	0.60
1:E:426:ASN:HB2	1:E:428:ASP:OD1	2.02	0.59
1:C:35:ARG:HB3	1:C:282:SER:HA	1.85	0.59
1:B:121:THR:HG23	1:B:139:TYR:HB2	1.83	0.59
1:C:245:MSE:H	1:C:254:ASN:ND2	2.01	0.59
1:C:354:ILE:HD12	1:C:354:ILE:N	2.17	0.59
1:E:103:ALA:CB	1:E:173:GLN:H	2.16	0.59
1:E:285:MSE:HG2	1:E:357:ILE:HG23	1.84	0.59
1:A:426:ASN:HB2	1:A:428:ASP:OD1	2.03	0.58
1:C:124:VAL:HG21	1:C:172:LEU:HD22	1.83	0.58
1:F:52:PHE:CE1	1:F:90:TYR:HB2	2.37	0.58
1:E:258:GLY:HA2	1:E:272:VAL:HG21	1.84	0.58
1:E:40:LEU:HD22	1:E:42:LEU:HG	1.84	0.58
1:C:324:ALA:CB	1:F:380:ASN:HB2	2.34	0.58
1:A:237:LYS:H	1:A:363:ASN:HD21	1.51	0.58
1:D:414:ASP:OD2	1:D:416:THR:HB	2.03	0.58
1:C:341:PHE:CD1	1:C:347:SER:HA	2.38	0.58
1:D:429:GLY:CA	1:D:452:LYS:HA	2.32	0.58
1:F:424:ASN:C	1:F:426:ASN:H	2.07	0.58
1:A:124:VAL:HG21	1:A:172:LEU:HD22	1.85	0.58
1:B:258:GLY:HA2	1:B:272:VAL:HG21	1.86	0.58
1:B:62:GLU:HA	1:B:67:LEU:O	2.04	0.58
1:D:285:MSE:HE1	1:D:404:LEU:HD13	1.85	0.58
1:D:102:LEU:HD11	1:D:122:ILE:CG2	2.33	0.58
1:A:48:ALA:O	1:A:49:ALA:HB3	2.03	0.58
1:B:48:ALA:O	1:B:49:ALA:HB3	2.02	0.58
1:C:426:ASN:HB2	1:C:428:ASP:OD1	2.04	0.58
1:B:285:MSE:HE2	1:B:409:ALA:HB1	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:GLY:HA3	1:A:281:ALA:O	2.03	0.57
1:F:55:ILE:O	1:F:55:ILE:HG13	2.04	0.57
1:B:102:LEU:HD11	1:B:122:ILE:CG2	2.33	0.57
1:D:50:LYS:NZ	1:D:195:GLN:HG3	2.19	0.57
1:E:424:ASN:C	1:E:426:ASN:H	2.08	0.57
1:A:248:ASP:HA	1:A:337:SER:O	2.03	0.57
1:E:237:LYS:HB2	1:E:363:ASN:ND2	2.18	0.57
1:A:118:ASN:HB3	1:B:179:THR:CG2	2.34	0.57
1:A:266:ILE:CD1	1:B:190:ASN:ND2	2.68	0.57
1:D:20:THR:O	1:D:24:ALA:HB2	2.04	0.57
1:F:426:ASN:HB2	1:F:428:ASP:OD1	2.04	0.57
1:E:341:PHE:CE1	1:E:347:SER:HA	2.39	0.57
1:A:334:ASP:OD2	1:A:356:ARG:NH2	2.31	0.57
1:E:22:PHE:CZ	1:E:368:ASN:HB3	2.40	0.57
1:B:424:ASN:C	1:B:426:ASN:H	2.08	0.57
1:A:340:THR:O	1:A:340:THR:HG23	2.05	0.57
1:D:424:ASN:C	1:D:426:ASN:H	2.08	0.57
1:E:285:MSE:HE1	1:E:361:ILE:HD11	1.87	0.56
1:E:102:LEU:HD11	1:E:122:ILE:CG2	2.33	0.56
1:B:23:LYS:NZ	1:B:403:GLU:HG2	2.20	0.56
1:D:61:VAL:HG21	1:D:69:LEU:HD13	1.87	0.56
1:A:373:ILE:HD12	1:A:453:LEU:HD23	1.85	0.56
1:F:102:LEU:HD11	1:F:122:ILE:CG2	2.35	0.56
1:A:18:ILE:O	1:A:21:ASN:HB2	2.05	0.56
1:B:369:ILE:O	1:B:373:ILE:HG12	2.05	0.56
1:A:343:LYS:HZ1	1:A:344:GLU:HG3	1.71	0.56
1:D:245:MSE:H	1:D:254:ASN:ND2	2.03	0.56
1:E:61:VAL:HG21	1:E:69:LEU:HD13	1.86	0.56
1:F:103:ALA:CB	1:F:173:GLN:H	2.18	0.56
1:E:48:ALA:O	1:E:49:ALA:HB3	2.05	0.56
1:E:363:ASN:N	1:E:363:ASN:HD22	2.03	0.56
1:F:50:LYS:NZ	1:F:195:GLN:HG3	2.21	0.56
1:C:258:GLY:HA2	1:C:272:VAL:HG21	1.87	0.56
1:A:43:ALA:HB1	1:A:93:ASN:ND2	2.20	0.56
1:A:103:ALA:CB	1:A:173:GLN:H	2.18	0.56
1:A:356:ARG:NH1	1:A:356:ARG:CG	2.65	0.56
1:A:424:ASN:C	1:A:426:ASN:H	2.10	0.56
1:B:50:LYS:NZ	1:B:195:GLN:HG3	2.21	0.56
1:D:103:ALA:CB	1:D:173:GLN:H	2.19	0.55
1:C:23:LYS:C	1:C:25:ALA:H	2.09	0.55
1:E:357:ILE:O	1:E:361:ILE:HG12	2.07	0.55
1:B:21:ASN:HD22	1:B:22:PHE:H	1.53	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:61:VAL:HG21	1:B:69:LEU:HD13	1.87	0.55
1:D:237:LYS:N	1:D:363:ASN:HD21	2.00	0.55
1:C:40:LEU:HD13	1:C:42:LEU:HD11	1.88	0.55
1:E:179:THR:HG23	1:F:118:ASN:HB3	1.89	0.55
1:C:29:ARG:HD2	1:C:35:ARG:HH22	1.71	0.55
1:A:290:THR:O	1:A:291:PHE:HB2	2.06	0.55
1:C:102:LEU:HD11	1:C:122:ILE:CG2	2.35	0.55
1:A:102:LEU:HD11	1:A:122:ILE:CG2	2.37	0.55
1:C:103:ALA:CB	1:C:173:GLN:H	2.18	0.55
1:C:424:ASN:C	1:C:426:ASN:H	2.09	0.55
1:A:245:MSE:H	1:A:254:ASN:ND2	2.05	0.55
1:F:62:GLU:HA	1:F:67:LEU:O	2.07	0.55
1:A:55:ILE:HG13	1:A:55:ILE:O	2.07	0.55
1:F:245:MSE:H	1:F:254:ASN:ND2	2.05	0.54
1:B:103:ALA:CB	1:B:173:GLN:H	2.19	0.54
1:F:124:VAL:HG13	1:F:175:SER:H	1.72	0.54
1:E:62:GLU:HA	1:E:67:LEU:O	2.07	0.54
1:F:122:ILE:N	1:F:122:ILE:HD12	2.22	0.54
1:E:52:PHE:CE1	1:E:90:TYR:HB2	2.41	0.54
1:F:48:ALA:O	1:F:49:ALA:HB3	2.07	0.54
1:D:345:LYS:HA	1:D:349:PHE:CE2	2.43	0.54
1:C:62:GLU:HA	1:C:67:LEU:O	2.07	0.54
1:C:55:ILE:HG13	1:C:55:ILE:O	2.08	0.54
1:B:248:ASP:HA	1:B:337:SER:O	2.07	0.54
1:F:35:ARG:NH1	1:F:284:SER:HA	2.22	0.54
1:F:45:SER:HB2	1:F:116:VAL:HG23	1.90	0.54
1:A:129:VAL:O	1:A:130:ASP:HB2	2.08	0.54
1:D:91:ARG:HD3	1:D:93:ASN:OD1	2.07	0.54
1:D:48:ALA:O	1:D:49:ALA:HB3	2.08	0.54
1:E:50:LYS:NZ	1:E:195:GLN:HG3	2.22	0.54
1:C:236:VAL:HG12	1:C:238:ILE:HG23	1.90	0.54
1:C:26:ALA:HB3	1:C:403:GLU:HB3	1.90	0.54
1:A:290:THR:HG23	1:A:333:GLN:HA	1.90	0.54
1:C:122:ILE:HD12	1:C:122:ILE:N	2.22	0.54
1:C:61:VAL:HG21	1:C:69:LEU:HD13	1.89	0.53
1:E:227:VAL:O	1:E:231:ARG:HG3	2.08	0.53
1:A:50:LYS:NZ	1:A:195:GLN:HG3	2.24	0.53
1:B:245:MSE:H	1:B:254:ASN:ND2	2.05	0.53
1:C:48:ALA:O	1:C:49:ALA:HB3	2.08	0.53
1:D:258:GLY:HA2	1:D:272:VAL:HG21	1.89	0.53
1:A:122:ILE:HD12	1:A:122:ILE:N	2.23	0.53
1:E:95:GLY:HA3	1:E:184:THR:O	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:227:VAL:O	1:F:231:ARG:HG3	2.08	0.53
1:E:122:ILE:HD12	1:E:122:ILE:N	2.23	0.53
1:B:324:ALA:HB2	1:C:380:ASN:HB2	1.91	0.53
1:B:237:LYS:H	1:B:363:ASN:HD21	1.57	0.53
1:C:391:GLN:NE2	1:C:394:LEU:HD23	2.24	0.53
1:A:233:GLU:HB2	1:C:229:ARG:CD	2.30	0.53
1:D:55:ILE:HG13	1:D:55:ILE:O	2.09	0.53
1:D:227:VAL:O	1:D:231:ARG:HG3	2.09	0.53
1:B:124:VAL:HG13	1:B:175:SER:H	1.72	0.53
1:E:391:GLN:NE2	1:E:394:LEU:HD23	2.24	0.53
1:D:122:ILE:HD12	1:D:122:ILE:N	2.24	0.53
1:A:124:VAL:HG13	1:A:175:SER:H	1.74	0.53
1:A:227:VAL:O	1:A:231:ARG:HG3	2.09	0.53
1:B:122:ILE:HD12	1:B:122:ILE:N	2.25	0.52
1:D:37:THR:CG2	1:D:86:THR:HB	2.39	0.52
1:C:220:LYS:HB3	1:C:245:MSE:HG3	1.91	0.52
1:B:348:LYS:HE3	1:B:441:SER:CB	2.40	0.52
1:F:129:VAL:O	1:F:130:ASP:HB2	2.09	0.52
1:D:124:VAL:HG13	1:D:175:SER:H	1.73	0.52
1:D:35:ARG:O	1:D:85:LYS:HB3	2.08	0.52
1:C:36:GLY:HA3	1:C:281:ALA:O	2.10	0.52
1:F:152:THR:HG22	1:F:155:GLU:HG3	1.92	0.52
1:D:236:VAL:HG12	1:D:238:ILE:HG23	1.91	0.52
1:E:38:VAL:HG21	1:E:277:ALA:HB1	1.91	0.52
1:C:152:THR:HG22	1:C:155:GLU:HG3	1.92	0.52
1:D:30:THR:HG23	1:D:286:LEU:HD11	1.92	0.52
1:D:345:LYS:HA	1:D:349:PHE:CD2	2.45	0.52
1:D:52:PHE:CE1	1:D:90:TYR:HB2	2.44	0.52
1:E:49:ALA:O	1:E:50:LYS:HB2	2.09	0.52
1:C:248:ASP:HA	1:C:337:SER:O	2.10	0.52
1:E:34:GLU:HB2	1:E:85:LYS:HD3	1.90	0.52
1:E:237:LYS:CB	1:E:363:ASN:HD21	2.22	0.52
1:C:35:ARG:CG	1:C:36:GLY:H	2.23	0.52
1:E:152:THR:CG2	1:E:155:GLU:HG3	2.39	0.52
1:A:129:VAL:O	1:A:129:VAL:HG12	2.10	0.52
1:C:50:LYS:NZ	1:C:195:GLN:HG3	2.24	0.52
1:C:124:VAL:HG13	1:C:175:SER:H	1.75	0.51
1:D:414:ASP:O	1:D:418:ASP:HB2	2.10	0.51
1:F:95:GLY:HA3	1:F:184:THR:O	2.10	0.51
1:C:41:PRO:HD3	1:C:196:PHE:CZ	2.46	0.51
1:F:369:ILE:CD1	1:F:393:ILE:HG23	2.40	0.51
1:E:334:ASP:C	1:E:352:ASN:HD22	2.13	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:152:THR:HG22	1:E:155:GLU:HG3	1.92	0.51
1:B:435:SER:HA	1:B:445:PHE:O	2.09	0.51
1:F:61:VAL:HG21	1:F:69:LEU:HD13	1.91	0.51
1:E:236:VAL:HG12	1:E:238:ILE:HG23	1.92	0.51
1:E:215:SER:CB	1:F:301:THR:HB	2.37	0.51
1:B:441:SER:O	1:B:443:GLU:N	2.43	0.51
1:F:236:VAL:HG12	1:F:238:ILE:HG23	1.93	0.51
1:D:30:THR:CG2	1:D:286:LEU:HD11	2.41	0.51
1:B:424:ASN:HD21	1:B:452:LYS:HE2	1.75	0.51
1:F:152:THR:CG2	1:F:155:GLU:HG3	2.40	0.51
1:D:34:GLU:HB3	1:D:85:LYS:HD3	1.92	0.51
1:D:62:GLU:HA	1:D:67:LEU:O	2.11	0.51
1:F:181:VAL:HG22	1:F:182:GLY:N	2.26	0.51
1:C:38:VAL:HA	1:C:207:THR:O	2.11	0.51
1:E:43:ALA:HB1	1:E:93:ASN:ND2	2.25	0.51
1:A:49:ALA:O	1:A:50:LYS:HB2	2.10	0.51
1:D:391:GLN:NE2	1:D:394:LEU:HD23	2.25	0.51
1:E:285:MSE:HE1	1:E:404:LEU:HD13	1.93	0.51
1:D:30:THR:HG23	1:D:286:LEU:CG	2.41	0.50
1:B:55:ILE:O	1:B:55:ILE:HG13	2.10	0.50
1:F:49:ALA:O	1:F:50:LYS:HB2	2.10	0.50
1:F:441:SER:O	1:F:443:GLU:N	2.44	0.50
1:C:435:SER:HA	1:C:445:PHE:O	2.11	0.50
1:A:248:ASP:OD2	1:A:340:THR:CG2	2.57	0.50
1:C:35:ARG:O	1:C:85:LYS:HB3	2.11	0.50
1:C:152:THR:CG2	1:C:155:GLU:HG3	2.41	0.50
1:E:124:VAL:HG13	1:E:175:SER:H	1.76	0.50
1:B:49:ALA:O	1:B:50:LYS:HB2	2.09	0.50
1:B:348:LYS:HE3	1:B:441:SER:HA	1.93	0.50
1:C:227:VAL:O	1:C:231:ARG:HG3	2.11	0.50
1:E:220:LYS:HB3	1:E:245:MSE:HG3	1.93	0.50
1:F:248:ASP:HA	1:F:337:SER:O	2.10	0.50
1:C:129:VAL:O	1:C:130:ASP:HB2	2.12	0.50
1:A:62:GLU:HA	1:A:67:LEU:O	2.12	0.50
1:C:23:LYS:HG2	1:C:403:GLU:HG3	1.92	0.50
1:B:152:THR:CG2	1:B:155:GLU:HG3	2.41	0.50
1:B:40:LEU:HD23	1:B:41:PRO:HD2	1.93	0.50
1:A:152:THR:HG22	1:A:155:GLU:HG3	1.94	0.50
1:C:414:ASP:O	1:C:418:ASP:HB2	2.12	0.50
1:F:43:ALA:HB1	1:F:93:ASN:ND2	2.26	0.50
1:D:34:GLU:CB	1:D:85:LYS:HD3	2.42	0.50
1:A:378:ASP:O	1:D:324:ALA:HB1	2.10	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:248:ASP:HA	1:D:337:SER:O	2.12	0.50
1:E:435:SER:HA	1:E:445:PHE:O	2.12	0.50
1:E:414:ASP:O	1:E:418:ASP:HB2	2.12	0.50
1:D:435:SER:HA	1:D:445:PHE:O	2.12	0.50
1:D:366:ARG:HB3	1:D:366:ARG:HH21	1.76	0.49
1:A:140:LEU:O	1:A:143:VAL:HG12	2.11	0.49
1:C:38:VAL:HG21	1:C:80:THR:HG21	1.94	0.49
1:E:190:ASN:HD21	1:F:266:ILE:HD11	1.76	0.49
1:B:341:PHE:CZ	1:B:350:ARG:HB2	2.47	0.49
1:D:95:GLY:HA3	1:D:184:THR:O	2.12	0.49
1:E:179:THR:CB	1:F:181:VAL:HG23	2.42	0.49
1:D:152:THR:HG22	1:D:155:GLU:HG3	1.94	0.49
1:C:46:TRP:HB2	1:C:116:VAL:HB	1.93	0.49
1:E:248:ASP:HA	1:E:337:SER:O	2.13	0.49
1:B:414:ASP:O	1:B:418:ASP:HB2	2.12	0.49
1:A:373:ILE:HD12	1:A:453:LEU:CD2	2.42	0.49
1:B:290:THR:HG23	1:B:333:GLN:HA	1.92	0.49
1:D:49:ALA:O	1:D:50:LYS:HB2	2.12	0.49
1:E:245:MSE:H	1:E:254:ASN:ND2	2.11	0.49
1:C:95:GLY:HA3	1:C:184:THR:O	2.12	0.49
1:A:341:PHE:CZ	1:A:350:ARG:HD3	2.46	0.49
1:B:30:THR:HB	1:B:286:LEU:HD11	1.94	0.49
1:E:45:SER:O	1:E:116:VAL:HG23	2.11	0.49
1:B:290:THR:O	1:B:291:PHE:CB	2.58	0.49
1:A:95:GLY:HA3	1:A:184:THR:O	2.13	0.49
1:E:333:GLN:NE2	1:E:335:LEU:HD21	2.28	0.49
1:A:336:ASN:HD22	1:A:336:ASN:C	2.16	0.49
1:B:152:THR:HG22	1:B:155:GLU:HG3	1.94	0.49
1:C:49:ALA:O	1:C:50:LYS:HB2	2.13	0.49
1:B:37:THR:HB	1:B:86:THR:HB	1.95	0.49
1:A:181:VAL:HG22	1:A:182:GLY:N	2.28	0.49
1:D:50:LYS:HZ3	1:D:195:GLN:HG3	1.78	0.49
1:D:390:VAL:HG13	1:D:421:VAL:HB	1.94	0.49
1:E:345:LYS:C	1:E:345:LYS:HD2	2.32	0.49
1:A:102:LEU:HD12	1:A:108:VAL:HG21	1.95	0.49
1:E:140:LEU:O	1:E:143:VAL:HG12	2.12	0.49
1:F:124:VAL:HG13	1:F:175:SER:N	2.28	0.49
1:F:356:ARG:CG	1:F:356:ARG:HH11	2.25	0.48
1:D:220:LYS:HB3	1:D:245:MSE:HG3	1.94	0.48
1:B:236:VAL:HG12	1:B:238:ILE:HG23	1.93	0.48
1:D:129:VAL:O	1:D:130:ASP:HB2	2.11	0.48
1:A:336:ASN:ND2	1:A:350:ARG:HA	2.27	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:152:THR:CG2	1:A:155:GLU:HG3	2.43	0.48
1:D:124:VAL:HG13	1:D:175:SER:N	2.28	0.48
1:B:124:VAL:HG13	1:B:175:SER:N	2.28	0.48
1:E:369:ILE:N	1:E:369:ILE:HD12	2.29	0.48
1:A:414:ASP:O	1:A:418:ASP:HB2	2.13	0.48
1:A:220:LYS:HB3	1:A:245:MSE:HG3	1.94	0.48
1:C:66:GLY:C	1:C:67:LEU:HD22	2.33	0.48
1:B:25:ALA:HA	1:B:28:GLU:HG2	1.96	0.48
1:F:391:GLN:NE2	1:F:394:LEU:HD23	2.27	0.48
1:C:30:THR:HB	1:C:286:LEU:CD1	2.41	0.48
1:B:52:PHE:CE1	1:B:90:TYR:HB2	2.48	0.48
1:A:127:ASN:HB3	1:A:130:ASP:O	2.14	0.48
1:F:129:VAL:HG12	1:F:129:VAL:O	2.13	0.48
1:D:23:LYS:HA	1:D:26:ALA:CB	2.44	0.48
1:E:290:THR:O	1:E:291:PHE:HB2	2.12	0.48
1:E:390:VAL:HG13	1:E:421:VAL:HB	1.94	0.48
1:B:129:VAL:O	1:B:130:ASP:HB2	2.13	0.48
1:B:21:ASN:HD22	1:B:22:PHE:N	2.11	0.48
1:B:324:ALA:CB	1:C:380:ASN:HB2	2.43	0.48
1:E:129:VAL:O	1:E:130:ASP:HB2	2.12	0.48
1:E:270:HIS:O	1:E:273:VAL:HG22	2.14	0.48
1:D:366:ARG:NH2	1:D:366:ARG:HB3	2.29	0.48
1:D:152:THR:CG2	1:D:155:GLU:HG3	2.43	0.48
1:F:71:HIS:CE1	1:F:73:SER:HG	2.32	0.48
1:B:227:VAL:O	1:B:231:ARG:HG3	2.13	0.48
1:F:435:SER:HA	1:F:445:PHE:O	2.14	0.48
1:E:37:THR:HA	1:E:86:THR:O	2.14	0.48
1:F:365:THR:O	1:F:369:ILE:HG12	2.14	0.48
1:C:102:LEU:HD12	1:C:108:VAL:HG21	1.96	0.48
1:D:181:VAL:HG22	1:D:182:GLY:N	2.28	0.48
1:D:285:MSE:HE3	1:D:357:ILE:HG23	1.96	0.47
1:E:179:THR:HB	1:F:181:VAL:HG23	1.96	0.47
1:A:435:SER:HA	1:A:445:PHE:O	2.14	0.47
1:F:454:GLU:HG3	1:F:454:GLU:O	2.14	0.47
1:D:237:LYS:HB3	1:D:359:ASP:OD2	2.14	0.47
1:B:220:LYS:HB3	1:B:245:MSE:HG3	1.95	0.47
1:B:354:ILE:HD12	1:B:354:ILE:H	1.79	0.47
1:F:102:LEU:HD12	1:F:108:VAL:HG21	1.95	0.47
1:E:50:LYS:HZ3	1:E:195:GLN:HG3	1.80	0.47
1:E:49:ALA:HA	1:E:91:ARG:HD3	1.96	0.47
1:B:95:GLY:HA3	1:B:184:THR:O	2.14	0.47
1:F:348:LYS:H	1:F:348:LYS:HD2	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:102:LEU:HD12	1:B:108:VAL:HG21	1.97	0.47
1:C:35:ARG:HH11	1:C:35:ARG:CG	2.26	0.47
1:B:23:LYS:HZ2	1:B:403:GLU:HG2	1.80	0.47
1:E:34:GLU:O	1:E:35:ARG:HG3	2.14	0.47
1:D:52:PHE:CD2	1:D:203:GLU:HG3	2.48	0.47
1:A:52:PHE:CE1	1:A:90:TYR:HB2	2.49	0.47
1:E:30:THR:HG23	1:E:286:LEU:CD1	2.35	0.47
1:B:140:LEU:O	1:B:143:VAL:HG12	2.14	0.47
1:A:266:ILE:HD13	1:B:190:ASN:ND2	2.28	0.47
1:F:414:ASP:O	1:F:418:ASP:HB2	2.14	0.47
1:F:45:SER:HB3	1:F:115:ILE:HG12	1.97	0.47
1:B:391:GLN:NE2	1:B:394:LEU:HD23	2.28	0.47
1:F:390:VAL:HG13	1:F:421:VAL:HB	1.95	0.47
1:C:57:LYS:HB3	1:C:59:GLU:OE2	2.15	0.47
1:A:40:LEU:O	1:A:89:VAL:HA	2.14	0.47
1:C:429:GLY:HA2	1:C:453:LEU:H	1.80	0.47
1:D:348:LYS:HD2	1:D:348:LYS:H	1.80	0.47
1:B:341:PHE:HZ	1:B:350:ARG:HB2	1.79	0.47
1:C:52:PHE:CD2	1:C:203:GLU:HG3	2.49	0.47
1:C:297:ALA:HB3	1:C:329:VAL:CG1	2.44	0.47
1:B:65:LEU:HD23	1:B:74:PHE:CE2	2.50	0.47
1:A:391:GLN:NE2	1:A:394:LEU:HD23	2.30	0.47
1:A:297:ALA:HB3	1:A:329:VAL:CG1	2.44	0.47
1:A:285:MSE:CE	1:A:357:ILE:HG23	2.31	0.47
1:F:52:PHE:CD2	1:F:203:GLU:HG3	2.50	0.47
1:B:19:TYR:C	1:B:21:ASN:H	2.18	0.47
1:C:52:PHE:CE1	1:C:90:TYR:HB2	2.50	0.47
1:E:55:ILE:HG13	1:E:55:ILE:O	2.14	0.47
1:F:334:ASP:OD2	1:F:352:ASN:HB2	2.15	0.47
1:E:353:LYS:O	1:E:357:ILE:HD11	2.14	0.47
1:A:333:GLN:NE2	1:A:335:LEU:HD21	2.30	0.47
1:F:23:LYS:HG2	1:F:403:GLU:CG	2.45	0.47
1:C:181:VAL:HG22	1:C:182:GLY:N	2.30	0.47
1:A:233:GLU:OE2	1:C:226:PHE:HA	2.15	0.47
1:E:354:ILE:O	1:E:357:ILE:HG12	2.15	0.47
1:B:50:LYS:HZ1	1:B:195:GLN:HG3	1.79	0.47
1:A:236:VAL:HG12	1:A:238:ILE:HG23	1.97	0.47
1:C:373:ILE:HD12	1:C:453:LEU:CD1	2.45	0.46
1:F:22:PHE:HZ	1:F:369:ILE:HD13	1.81	0.46
1:F:333:GLN:NE2	1:F:335:LEU:HD21	2.30	0.46
1:A:35:ARG:HB3	1:A:282:SER:HA	1.97	0.46
1:F:140:LEU:O	1:F:143:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:356:ARG:HG2	1:F:356:ARG:NH1	2.28	0.46
1:A:124:VAL:HG13	1:A:175:SER:N	2.30	0.46
1:C:424:ASN:HD21	1:C:452:LYS:NZ	2.12	0.46
1:D:441:SER:O	1:D:443:GLU:N	2.46	0.46
1:A:181:VAL:HG23	1:B:179:THR:CG2	2.45	0.46
1:C:38:VAL:HG12	1:C:281:ALA:CB	2.45	0.46
1:D:333:GLN:NE2	1:D:335:LEU:HD21	2.30	0.46
1:F:43:ALA:HB1	1:F:93:ASN:HD22	1.80	0.46
1:C:100:ALA:HB2	1:C:180:LEU:HA	1.96	0.46
1:C:35:ARG:CG	1:C:35:ARG:NH1	2.78	0.46
1:C:441:SER:O	1:C:443:GLU:N	2.48	0.46
1:E:180:LEU:HD12	1:E:180:LEU:N	2.31	0.46
1:D:41:PRO:HG2	1:D:41:PRO:O	2.15	0.46
1:A:369:ILE:HD12	1:A:393:ILE:HG23	1.98	0.46
1:D:129:VAL:HG12	1:D:129:VAL:O	2.16	0.46
1:E:441:SER:O	1:E:443:GLU:N	2.49	0.46
1:E:52:PHE:CD2	1:E:203:GLU:HG3	2.49	0.46
1:F:35:ARG:HH11	1:F:284:SER:HA	1.81	0.46
1:C:71:HIS:CE1	1:C:73:SER:HG	2.34	0.46
1:D:46:TRP:HB2	1:D:116:VAL:HB	1.98	0.46
1:C:333:GLN:NE2	1:C:335:LEU:HD21	2.31	0.46
1:A:71:HIS:ND1	1:A:72:GLN:N	2.64	0.46
1:E:214:SER:HA	1:E:220:LYS:NZ	2.30	0.46
1:C:390:VAL:HG13	1:C:421:VAL:HB	1.97	0.46
1:E:71:HIS:CE1	1:E:73:SER:HG	2.34	0.46
1:A:390:VAL:HG13	1:A:421:VAL:HB	1.98	0.46
1:A:180:LEU:N	1:A:180:LEU:HD12	2.30	0.46
1:C:140:LEU:O	1:C:143:VAL:HG12	2.16	0.46
1:B:66:GLY:C	1:B:67:LEU:HD22	2.37	0.46
1:B:52:PHE:CD2	1:B:203:GLU:HG3	2.50	0.46
1:A:210:PHE:HB3	1:A:242:VAL:CG1	2.46	0.46
1:B:288:SER:OG	1:B:289:ASN:N	2.48	0.46
1:C:124:VAL:HG13	1:C:175:SER:N	2.30	0.46
1:D:127:ASN:HB3	1:D:130:ASP:O	2.15	0.46
1:D:23:LYS:HE2	1:D:399:ALA:HB1	1.98	0.46
1:E:181:VAL:HG22	1:E:182:GLY:N	2.31	0.46
1:E:102:LEU:HD12	1:E:108:VAL:HG21	1.97	0.45
1:E:66:GLY:C	1:E:67:LEU:HD22	2.36	0.45
1:C:237:LYS:H	1:C:363:ASN:HD21	1.64	0.45
1:B:362:ASN:HB2	1:B:447:PHE:CD2	2.51	0.45
1:F:71:HIS:ND1	1:F:72:GLN:N	2.64	0.45
1:D:297:ALA:HB3	1:D:329:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:336:ASN:HD22	1:F:336:ASN:C	2.19	0.45
1:E:336:ASN:HD22	1:E:336:ASN:C	2.19	0.45
1:B:45:SER:O	1:B:116:VAL:HG23	2.17	0.45
1:E:129:VAL:HG12	1:E:129:VAL:O	2.17	0.45
1:C:288:SER:OG	1:C:289:ASN:N	2.49	0.45
1:B:390:VAL:HG13	1:B:421:VAL:HB	1.98	0.45
1:B:34:GLU:HB3	1:B:85:LYS:HD3	1.99	0.45
1:D:367:ARG:HG2	1:D:367:ARG:HH21	1.81	0.45
1:C:103:ALA:HB2	1:C:173:GLN:O	2.17	0.45
1:B:341:PHE:CD1	1:B:347:SER:HA	2.52	0.45
1:F:297:ALA:HB3	1:F:329:VAL:CG1	2.46	0.45
1:D:361:ILE:CD1	1:D:436:ILE:HG21	2.47	0.45
1:B:180:LEU:N	1:B:180:LEU:HD12	2.31	0.45
1:C:29:ARG:HA	1:C:35:ARG:CZ	2.45	0.45
1:A:414:ASP:O	1:A:416:THR:N	2.49	0.45
1:C:288:SER:HB2	1:C:353:LYS:HD2	1.97	0.45
1:A:441:SER:O	1:A:443:GLU:N	2.50	0.45
1:F:180:LEU:HD12	1:F:180:LEU:N	2.31	0.45
1:D:100:ALA:HB2	1:D:180:LEU:HA	1.98	0.45
1:A:366:ARG:HG3	1:A:367:ARG:N	2.32	0.45
1:F:369:ILE:HD12	1:F:393:ILE:HG23	1.98	0.45
1:C:129:VAL:O	1:C:129:VAL:HG12	2.16	0.45
1:E:297:ALA:HB3	1:E:329:VAL:CG1	2.46	0.45
1:D:44:ALA:HB3	1:D:91:ARG:CG	2.41	0.45
1:A:122:ILE:HD11	1:A:162:VAL:HG11	1.99	0.45
1:B:248:ASP:CG	1:B:340:THR:HG22	2.36	0.45
1:B:210:PHE:HB3	1:B:242:VAL:CG1	2.47	0.45
1:A:45:SER:O	1:A:46:TRP:HB2	2.17	0.45
1:B:99:THR:CG2	1:B:100:ALA:H	2.23	0.45
1:D:102:LEU:HD12	1:D:108:VAL:HG21	1.98	0.45
1:E:340:THR:O	1:E:340:THR:HG23	2.17	0.45
1:A:361:ILE:HG22	1:A:362:ASN:N	2.31	0.45
1:F:100:ALA:HB2	1:F:180:LEU:HA	1.98	0.45
1:D:23:LYS:C	1:D:25:ALA:H	2.21	0.45
1:E:127:ASN:HB3	1:E:130:ASP:O	2.16	0.45
1:F:289:ASN:HD22	1:F:289:ASN:HA	1.55	0.45
1:B:71:HIS:ND1	1:B:72:GLN:N	2.65	0.45
1:E:347:SER:C	1:E:349:PHE:H	2.20	0.44
1:C:18:ILE:HD12	1:C:18:ILE:N	2.30	0.44
1:A:71:HIS:CE1	1:A:73:SER:HG	2.35	0.44
1:B:311:GLU:O	1:B:314:GLN:HB3	2.17	0.44
1:F:65:LEU:HD23	1:F:74:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:135:ASP:OD2	1:F:149:VAL:HG22	2.17	0.44
1:C:336:ASN:C	1:C:336:ASN:HD22	2.20	0.44
1:A:29:ARG:HD2	1:A:285:MSE:SE	2.66	0.44
1:C:38:VAL:HG21	1:C:80:THR:CG2	2.47	0.44
1:B:129:VAL:O	1:B:129:VAL:HG12	2.16	0.44
1:C:71:HIS:ND1	1:C:72:GLN:N	2.65	0.44
1:B:297:ALA:HB3	1:B:329:VAL:CG1	2.47	0.44
1:E:57:LYS:HB3	1:E:59:GLU:OE2	2.17	0.44
1:D:71:HIS:ND1	1:D:72:GLN:N	2.65	0.44
1:B:437:GLU:HB2	1:B:444:LYS:HG2	1.98	0.44
1:E:311:GLU:O	1:E:314:GLN:HB3	2.18	0.44
1:B:303:ARG:C	1:B:304:LEU:HD12	2.38	0.44
1:D:30:THR:HG23	1:D:286:LEU:HG	1.99	0.44
1:D:285:MSE:O	1:D:357:ILE:HD11	2.18	0.44
1:B:122:ILE:HD11	1:B:162:VAL:HG11	1.99	0.44
1:C:29:ARG:CA	1:C:35:ARG:NH2	2.80	0.44
1:E:288:SER:HB2	1:E:353:LYS:HG2	1.99	0.44
1:E:124:VAL:HG13	1:E:175:SER:N	2.32	0.44
1:B:333:GLN:NE2	1:B:335:LEU:HD21	2.32	0.44
1:D:140:LEU:O	1:D:143:VAL:HG12	2.17	0.44
1:D:336:ASN:HD22	1:D:336:ASN:C	2.20	0.44
1:D:36:GLY:HA3	1:D:281:ALA:O	2.16	0.44
1:A:29:ARG:HB3	1:A:285:MSE:SE	2.68	0.44
1:C:373:ILE:HD12	1:C:453:LEU:HD12	1.98	0.44
1:B:49:ALA:HA	1:B:91:ARG:HD3	2.00	0.44
1:D:351:LYS:NZ	1:D:353:LYS:HB3	2.32	0.44
1:A:100:ALA:HB2	1:A:180:LEU:HA	1.99	0.44
1:B:21:ASN:HD22	1:B:21:ASN:N	2.15	0.44
1:C:40:LEU:HD13	1:C:42:LEU:CD1	2.48	0.44
1:A:288:SER:OG	1:A:289:ASN:N	2.51	0.44
1:C:245:MSE:H	1:C:254:ASN:HD21	1.65	0.44
1:D:71:HIS:CE1	1:D:73:SER:HG	2.35	0.44
1:B:433:ASN:HD22	1:B:433:ASN:N	2.14	0.44
1:F:343:LYS:HG3	1:F:344:GLU:N	2.33	0.44
1:B:414:ASP:C	1:B:416:THR:N	2.71	0.44
1:A:414:ASP:C	1:A:416:THR:N	2.71	0.44
1:D:360:GLY:O	1:D:361:ILE:C	2.55	0.44
1:B:336:ASN:C	1:B:336:ASN:HD22	2.22	0.44
1:F:189:THR:HG23	1:F:192:ASP:CG	2.38	0.44
1:A:26:ALA:HB2	1:A:400:TYR:CD1	2.53	0.44
1:B:42:LEU:HD12	1:B:89:VAL:HG23	1.99	0.44
1:F:127:ASN:HB3	1:F:130:ASP:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:GLY:C	1:A:67:LEU:HD22	2.39	0.44
1:E:71:HIS:ND1	1:E:72:GLN:N	2.66	0.44
1:C:194:THR:O	1:C:198:VAL:HG23	2.18	0.44
1:A:433:ASN:N	1:A:433:ASN:HD22	2.15	0.44
1:E:285:MSE:HE3	1:E:357:ILE:HG23	2.00	0.43
1:C:354:ILE:CD1	1:C:354:ILE:N	2.80	0.43
1:C:452:LYS:O	1:C:454:GLU:N	2.50	0.43
1:C:50:LYS:HZ1	1:C:195:GLN:HG3	1.82	0.43
1:B:127:ASN:HB3	1:B:130:ASP:O	2.18	0.43
1:D:285:MSE:HG2	1:D:357:ILE:CG1	2.39	0.43
1:E:99:THR:CG2	1:E:100:ALA:H	2.21	0.43
1:D:180:LEU:N	1:D:180:LEU:HD12	2.33	0.43
1:F:50:LYS:HZ3	1:F:195:GLN:HG3	1.82	0.43
1:D:400:TYR:HD2	1:D:401:LEU:HD22	1.83	0.43
1:E:400:TYR:HD2	1:E:401:LEU:HD22	1.84	0.43
1:C:270:HIS:O	1:C:273:VAL:HG22	2.18	0.43
1:A:438:PRO:O	1:A:439:VAL:C	2.56	0.43
1:B:41:PRO:HB3	1:B:196:PHE:CD1	2.53	0.43
1:C:41:PRO:HG2	1:C:41:PRO:O	2.19	0.43
1:F:270:HIS:O	1:F:273:VAL:HG22	2.18	0.43
1:C:135:ASP:OD2	1:C:149:VAL:HG22	2.17	0.43
1:F:57:LYS:HB3	1:F:59:GLU:OE2	2.17	0.43
1:A:414:ASP:C	1:A:416:THR:H	2.22	0.43
1:E:65:LEU:HD23	1:E:74:PHE:CE2	2.52	0.43
1:C:99:THR:CG2	1:C:100:ALA:N	2.82	0.43
1:B:100:ALA:HB2	1:B:180:LEU:HA	2.00	0.43
1:D:290:THR:O	1:D:291:PHE:CB	2.66	0.43
1:A:43:ALA:HB1	1:A:93:ASN:HD22	1.82	0.43
1:D:66:GLY:C	1:D:67:LEU:HD22	2.39	0.43
1:E:220:LYS:HD3	1:E:245:MSE:HG2	2.01	0.43
1:C:127:ASN:HB3	1:C:130:ASP:O	2.18	0.43
1:C:342:SER:OG	1:C:343:LYS:N	2.51	0.43
1:F:42:LEU:HD23	1:F:42:LEU:HA	1.77	0.43
1:A:229:ARG:HD2	1:C:201:GLU:OE1	2.19	0.43
1:F:414:ASP:O	1:F:416:THR:N	2.50	0.43
1:E:433:ASN:N	1:E:433:ASN:HD22	2.16	0.43
1:D:122:ILE:HD11	1:D:162:VAL:HG11	2.01	0.43
1:C:414:ASP:C	1:C:416:THR:N	2.72	0.43
1:F:220:LYS:HB3	1:F:245:MSE:HG3	2.00	0.43
1:B:181:VAL:HG22	1:B:182:GLY:N	2.34	0.43
1:E:103:ALA:HB1	1:E:173:GLN:N	2.31	0.43
1:B:220:LYS:HD3	1:B:245:MSE:HG2	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:376:ARG:HD2	1:E:376:ARG:HA	1.80	0.43
1:A:400:TYR:HD2	1:A:401:LEU:HD22	1.84	0.43
1:C:229:ARG:O	1:C:230:MSE:C	2.57	0.43
1:F:40:LEU:HD23	1:F:41:PRO:N	2.34	0.43
1:F:49:ALA:HA	1:F:91:ARG:HD3	2.00	0.43
1:C:49:ALA:HA	1:C:91:ARG:HD3	2.01	0.43
1:A:35:ARG:O	1:A:36:GLY:O	2.37	0.42
1:E:319:VAL:HG23	1:E:332:GLU:CB	2.44	0.42
1:B:140:LEU:O	1:B:141:ASN:CB	2.62	0.42
1:B:414:ASP:O	1:B:416:THR:N	2.52	0.42
1:A:30:THR:HG21	1:A:407:SER:OG	2.18	0.42
1:D:30:THR:HG23	1:D:286:LEU:CD1	2.49	0.42
1:E:345:LYS:HB2	1:E:349:PHE:CD2	2.54	0.42
1:E:21:ASN:HD22	1:E:22:PHE:H	1.62	0.42
1:F:66:GLY:C	1:F:67:LEU:HD22	2.40	0.42
1:A:308:GLU:O	1:A:311:GLU:HB3	2.19	0.42
1:C:180:LEU:N	1:C:180:LEU:HD12	2.35	0.42
1:D:438:PRO:O	1:D:439:VAL:C	2.57	0.42
1:B:48:ALA:O	1:B:49:ALA:CB	2.67	0.42
1:B:194:THR:O	1:B:198:VAL:HG23	2.19	0.42
1:A:99:THR:O	1:A:100:ALA:HB2	2.19	0.42
1:B:438:PRO:O	1:B:439:VAL:C	2.58	0.42
1:C:35:ARG:HG2	1:C:36:GLY:H	1.84	0.42
1:E:333:GLN:CD	1:E:335:LEU:HD21	2.38	0.42
1:D:335:LEU:HD22	1:D:350:ARG:HD3	2.01	0.42
1:A:65:LEU:HD23	1:A:74:PHE:CE2	2.55	0.42
1:B:103:ALA:HB2	1:B:173:GLN:O	2.20	0.42
1:E:336:ASN:ND2	1:E:338:LEU:HB3	2.33	0.42
1:F:119:SER:HB3	1:F:141:ASN:HD21	1.82	0.42
1:D:103:ALA:HB2	1:D:173:GLN:O	2.19	0.42
1:D:336:ASN:HD21	1:D:350:ARG:HA	1.85	0.42
1:B:33:GLY:O	1:B:34:GLU:C	2.58	0.42
1:C:255:VAL:HG21	1:C:273:VAL:HG12	2.01	0.42
1:F:243:ALA:HB2	1:F:270:HIS:HA	2.02	0.42
1:C:437:GLU:HB2	1:C:444:LYS:HG2	2.01	0.42
1:C:21:ASN:HA	1:C:24:ALA:HB3	2.01	0.42
1:E:308:GLU:O	1:E:311:GLU:HB3	2.19	0.42
1:B:400:TYR:HD2	1:B:401:LEU:HD22	1.85	0.42
1:D:437:GLU:HB2	1:D:444:LYS:HG2	2.01	0.42
1:F:433:ASN:N	1:F:433:ASN:HD22	2.17	0.42
1:F:99:THR:O	1:F:100:ALA:HB2	2.20	0.42
1:D:366:ARG:CG	1:D:367:ARG:N	2.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:103:ALA:HB2	1:E:173:GLN:O	2.20	0.42
1:F:102:LEU:HD23	1:F:103:ALA:H	1.85	0.42
1:E:369:ILE:HD12	1:E:369:ILE:H	1.85	0.42
1:C:438:PRO:O	1:C:439:VAL:C	2.58	0.42
1:E:414:ASP:C	1:E:416:THR:N	2.73	0.42
1:C:414:ASP:O	1:C:416:THR:N	2.52	0.42
1:B:336:ASN:ND2	1:B:338:LEU:HB3	2.35	0.42
1:F:57:LYS:O	1:F:60:ASP:HB2	2.20	0.42
1:A:437:GLU:HB2	1:A:444:LYS:HG2	2.02	0.42
1:C:400:TYR:HD2	1:C:401:LEU:HD22	1.85	0.42
1:D:285:MSE:HE2	1:D:409:ALA:CB	2.44	0.42
1:B:103:ALA:HB1	1:B:173:GLN:CB	2.46	0.42
1:E:336:ASN:ND2	1:E:350:ARG:HA	2.30	0.42
1:F:122:ILE:HD11	1:F:162:VAL:HG11	2.02	0.42
1:C:23:LYS:C	1:C:25:ALA:N	2.72	0.42
1:C:26:ALA:CB	1:C:403:GLU:HB3	2.49	0.42
1:D:369:ILE:O	1:D:373:ILE:HG12	2.19	0.42
1:C:45:SER:O	1:C:46:TRP:HB2	2.19	0.42
1:D:207:THR:HG22	1:D:208:ILE:N	2.35	0.42
1:A:358:LEU:O	1:A:359:ASP:C	2.56	0.42
1:E:437:GLU:HB2	1:E:444:LYS:HG2	2.02	0.42
1:A:119:SER:HB3	1:A:141:ASN:HD21	1.84	0.42
1:A:18:ILE:O	1:A:21:ASN:N	2.50	0.42
1:B:30:THR:HG21	1:B:407:SER:OG	2.19	0.42
1:E:40:LEU:O	1:E:89:VAL:HA	2.20	0.42
1:F:33:GLY:O	1:F:35:ARG:HG2	2.20	0.42
1:F:333:GLN:CD	1:F:335:LEU:HD21	2.40	0.42
1:F:437:GLU:HB2	1:F:444:LYS:HG2	2.02	0.42
1:D:210:PHE:HB3	1:D:242:VAL:CG1	2.49	0.42
1:F:210:PHE:HB3	1:F:242:VAL:CG1	2.50	0.42
1:F:308:GLU:O	1:F:311:GLU:HB3	2.19	0.42
1:E:122:ILE:HD11	1:E:162:VAL:HG11	2.02	0.42
1:C:30:THR:HG21	1:C:407:SER:OG	2.18	0.42
1:F:438:PRO:O	1:F:439:VAL:C	2.58	0.42
1:A:49:ALA:HA	1:A:91:ARG:HD3	2.01	0.42
1:A:294:TYR:HB3	1:A:329:VAL:HG13	2.01	0.42
1:B:71:HIS:CE1	1:B:73:SER:HG	2.37	0.42
1:D:433:ASN:HD22	1:D:433:ASN:N	2.15	0.42
1:B:119:SER:HB3	1:B:141:ASN:HD21	1.85	0.41
1:C:23:LYS:HG2	1:C:403:GLU:CG	2.50	0.41
1:F:414:ASP:C	1:F:416:THR:N	2.71	0.41
1:A:245:MSE:H	1:A:254:ASN:HD21	1.67	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:52:PHE:CD2	1:A:203:GLU:HG3	2.54	0.41
1:E:194:THR:O	1:E:198:VAL:HG23	2.20	0.41
1:B:235:GLY:C	1:B:366:ARG:HH12	2.22	0.41
1:A:381:THR:O	1:A:382:ASP:C	2.59	0.41
1:C:65:LEU:HD23	1:C:74:PHE:CE2	2.55	0.41
1:D:355:SER:O	1:D:359:ASP:HB2	2.20	0.41
1:D:38:VAL:HA	1:D:207:THR:O	2.20	0.41
1:D:311:GLU:O	1:D:314:GLN:HB3	2.20	0.41
1:A:194:THR:O	1:A:198:VAL:HG23	2.20	0.41
1:A:285:MSE:O	1:A:357:ILE:HD11	2.20	0.41
1:D:20:THR:C	1:D:24:ALA:HB2	2.41	0.41
1:A:333:GLN:CD	1:A:335:LEU:HD21	2.41	0.41
1:F:255:VAL:HG21	1:F:273:VAL:HG12	2.01	0.41
1:B:102:LEU:HD23	1:B:103:ALA:H	1.85	0.41
1:C:119:SER:HB3	1:C:141:ASN:HD21	1.82	0.41
1:E:294:TYR:HB3	1:E:329:VAL:HG13	2.03	0.41
1:A:301:THR:HA	1:A:302:PRO:HA	1.92	0.41
1:E:36:GLY:HA3	1:E:281:ALA:O	2.20	0.41
1:C:37:THR:HG22	1:C:86:THR:HB	2.03	0.41
1:B:273:VAL:HG23	1:B:274:ALA:N	2.35	0.41
1:A:26:ALA:O	1:A:29:ARG:HB2	2.20	0.41
1:F:256:ARG:HB3	1:F:319:VAL:HG12	2.01	0.41
1:C:38:VAL:HG12	1:C:281:ALA:HB2	2.03	0.41
1:C:34:GLU:HB3	1:C:85:LYS:HB2	2.02	0.41
1:F:414:ASP:C	1:F:416:THR:H	2.24	0.41
1:A:50:LYS:HZ1	1:A:195:GLN:HG3	1.85	0.41
1:C:364:ASP:O	1:C:368:ASN:HB2	2.21	0.41
1:B:57:LYS:HB3	1:B:59:GLU:OE2	2.20	0.41
1:E:100:ALA:HB2	1:E:180:LEU:HA	2.03	0.41
1:E:99:THR:O	1:E:100:ALA:HB2	2.21	0.41
1:B:26:ALA:HB1	1:B:403:GLU:HB3	2.02	0.41
1:D:245:MSE:H	1:D:254:ASN:HD21	1.68	0.41
1:B:294:TYR:HB3	1:B:329:VAL:HG13	2.02	0.41
1:D:194:THR:O	1:D:198:VAL:HG23	2.20	0.41
1:B:354:ILE:HD12	1:B:354:ILE:N	2.35	0.41
1:B:229:ARG:O	1:B:230:MSE:C	2.59	0.41
1:C:299:ASP:OD1	1:C:303:ARG:NH2	2.54	0.41
1:E:106:VAL:O	1:E:108:VAL:HG23	2.20	0.41
1:E:438:PRO:O	1:E:439:VAL:C	2.58	0.41
1:C:25:ALA:O	1:C:28:GLU:HB2	2.21	0.41
1:F:373:ILE:HD12	1:F:453:LEU:HD12	2.02	0.41
1:C:210:PHE:HB3	1:C:242:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:57:LYS:O	1:D:60:ASP:HB2	2.20	0.41
1:E:210:PHE:HB3	1:E:242:VAL:CG1	2.51	0.41
1:A:189:THR:HG23	1:A:192:ASP:CG	2.41	0.41
1:A:135:ASP:OD2	1:A:149:VAL:HG22	2.20	0.41
1:D:351:LYS:NZ	1:D:351:LYS:HB3	2.35	0.41
1:C:99:THR:O	1:C:100:ALA:HB2	2.20	0.41
1:B:99:THR:CG2	1:B:100:ALA:N	2.81	0.41
1:D:103:ALA:HB1	1:D:173:GLN:CB	2.47	0.41
1:C:29:ARG:N	1:C:35:ARG:NH2	2.68	0.41
1:B:41:PRO:HD3	1:B:196:PHE:CZ	2.56	0.41
1:B:124:VAL:HG12	1:B:175:SER:HB3	2.03	0.41
1:E:220:LYS:HB3	1:E:245:MSE:CG	2.51	0.41
1:F:336:ASN:HD21	1:F:350:ARG:HA	1.85	0.41
1:C:368:ASN:HD22	1:C:368:ASN:HA	1.64	0.41
1:C:367:ARG:HH21	1:C:368:ASN:HD21	1.69	0.41
1:C:300:ALA:O	1:C:303:ARG:HG3	2.21	0.41
1:C:433:ASN:HD22	1:C:433:ASN:N	2.17	0.41
1:E:179:THR:HG22	1:F:181:VAL:CG2	2.47	0.41
1:F:237:LYS:HB2	1:F:363:ASN:HD21	1.82	0.41
1:D:414:ASP:C	1:D:416:THR:N	2.74	0.41
1:E:243:ALA:HB2	1:E:270:HIS:HA	2.03	0.41
1:D:124:VAL:HG21	1:D:172:LEU:CD2	2.49	0.40
1:C:414:ASP:C	1:C:416:THR:H	2.24	0.40
1:F:23:LYS:HG2	1:F:403:GLU:HG3	2.03	0.40
1:F:294:TYR:HB3	1:F:329:VAL:HG13	2.02	0.40
1:B:57:LYS:O	1:B:60:ASP:HB2	2.21	0.40
1:E:210:PHE:HB2	1:E:223:PHE:CZ	2.56	0.40
1:D:288:SER:OG	1:D:289:ASN:N	2.54	0.40
1:F:143:VAL:HG13	1:F:143:VAL:O	2.20	0.40
1:F:356:ARG:CG	1:F:356:ARG:NH1	2.84	0.40
1:D:414:ASP:O	1:D:416:THR:N	2.54	0.40
1:C:231:ARG:HD3	1:C:249:TYR:OH	2.21	0.40
1:E:189:THR:HG23	1:E:192:ASP:CG	2.42	0.40
1:F:26:ALA:HB2	1:F:400:TYR:CD1	2.56	0.40
1:D:99:THR:O	1:D:100:ALA:HB2	2.21	0.40
1:E:45:SER:O	1:E:46:TRP:CB	2.66	0.40
1:F:189:THR:HG23	1:F:192:ASP:OD2	2.20	0.40
1:B:99:THR:O	1:B:100:ALA:HB2	2.21	0.40
1:E:102:LEU:HD23	1:E:103:ALA:H	1.86	0.40
1:A:247:ALA:O	1:A:248:ASP:C	2.59	0.40
1:B:143:VAL:HG13	1:B:143:VAL:O	2.21	0.40
1:A:18:ILE:CD1	1:A:372:ALA:HA	2.50	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:414:ASP:O	1:E:416:THR:N	2.54	0.40
1:C:40:LEU:HD23	1:C:41:PRO:HD2	2.02	0.40
1:D:247:ALA:O	1:D:248:ASP:C	2.60	0.40
1:B:251:GLY:O	1:B:252:ILE:HD12	2.21	0.40
1:E:231:ARG:HD3	1:E:249:TYR:OH	2.22	0.40
1:F:336:ASN:ND2	1:F:338:LEU:HB3	2.37	0.40
1:B:189:THR:HG23	1:B:192:ASP:CG	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	438/460 (95%)	372 (85%)	54 (12%)	12 (3%)	8	49
1	B	433/460 (94%)	370 (86%)	53 (12%)	10 (2%)	10	54
1	C	436/460 (95%)	371 (85%)	51 (12%)	14 (3%)	6	43
1	D	432/460 (94%)	359 (83%)	60 (14%)	13 (3%)	7	46
1	E	429/460 (93%)	370 (86%)	45 (10%)	14 (3%)	6	43
1	F	433/460 (94%)	373 (86%)	48 (11%)	12 (3%)	8	48
All	All	2601/2760 (94%)	2215 (85%)	311 (12%)	75 (3%)	7	47

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLY
1	A	130	ASP
1	A	439	VAL
1	B	130	ASP
1	B	439	VAL
1	C	36	GLY
1	C	130	ASP
1	C	439	VAL

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Mol	Chain	Res	Type
1	D	36	GLY
1	D	130	ASP
1	D	439	VAL
1	D	452	LYS
1	E	130	ASP
1	E	439	VAL
1	F	130	ASP
1	F	439	VAL
1	A	103	ALA
1	A	215	SER
1	A	424	ASN
1	B	103	ALA
1	B	215	SER
1	B	424	ASN
1	B	442	GLY
1	C	103	ALA
1	C	215	SER
1	C	424	ASN
1	C	453	LEU
1	D	103	ALA
1	D	215	SER
1	D	424	ASN
1	E	31	LYS
1	E	103	ALA
1	E	215	SER
1	E	424	ASN
1	F	103	ALA
1	F	215	SER
1	F	424	ASN
1	F	442	GLY
1	A	415	SER
1	A	442	GLY
1	B	415	SER
1	C	46	TRP
1	C	441	SER
1	D	441	SER
1	D	442	GLY
1	F	415	SER
1	F	441	SER
1	A	244	ASN
1	A	441	SER
1	B	34	GLU

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Mol	Chain	Res	Type
1	B	441	SER
1	C	24	ALA
1	C	415	SER
1	C	442	GLY
1	D	415	SER
1	E	46	TRP
1	E	244	ASN
1	E	348	LYS
1	E	415	SER
1	E	441	SER
1	F	346	SER
1	A	49	ALA
1	C	49	ALA
1	D	25	ALA
1	D	49	ALA
1	E	49	ALA
1	E	442	GLY
1	F	49	ALA
1	F	244	ASN
1	A	19	TYR
1	B	244	ASN
1	D	177	GLY
1	C	177	GLY
1	F	177	GLY
1	E	177	GLY

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	372/383 (97%)	332 (89%)	40 (11%)	9	39
1	B	368/383 (96%)	329 (89%)	39 (11%)	10	40
1	C	370/383 (97%)	329 (89%)	41 (11%)	9	37
1	D	367/383 (96%)	327 (89%)	40 (11%)	9	38
1	E	364/383 (95%)	320 (88%)	44 (12%)	7	33
1	F	368/383 (96%)	325 (88%)	43 (12%)	8	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2209/2298 (96%)	1962 (89%)	247 (11%)	9 37

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	37	THR
1	A	38	VAL
1	A	40	LEU
1	A	56	ASN
1	A	65	LEU
1	A	75	LEU
1	A	102	LEU
1	A	121	THR
1	A	127	ASN
1	A	137	THR
1	A	142	GLU
1	A	172	LEU
1	A	174	GLN
1	A	178	THR
1	A	179	THR
1	A	185	ASP
1	A	189	THR
1	A	191	LEU
1	A	242	VAL
1	A	245	MSE
1	A	280	ASP
1	A	284	SER
1	A	285	MSE
1	A	287	LYS
1	A	294	TYR
1	A	307	ASP
1	A	325	ARG
1	A	333	GLN
1	A	336	ASN
1	A	347	SER
1	A	363	ASN
1	A	366	ARG
1	A	375	GLU
1	A	376	ARG
1	A	380	ASN
1	A	381	THR

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Mol	Chain	Res	Type
1	A	391	GLN
1	A	447	PHE
1	A	448	THR
1	B	21	ASN
1	B	35	ARG
1	B	37	THR
1	B	38	VAL
1	B	40	LEU
1	B	56	ASN
1	B	65	LEU
1	B	75	LEU
1	B	102	LEU
1	B	121	THR
1	B	127	ASN
1	B	137	THR
1	B	142	GLU
1	B	172	LEU
1	B	174	GLN
1	B	178	THR
1	B	179	THR
1	B	185	ASP
1	B	189	THR
1	B	191	LEU
1	B	230	MSE
1	B	242	VAL
1	B	245	MSE
1	B	280	ASP
1	B	285	MSE
1	B	287	LYS
1	B	294	TYR
1	B	307	ASP
1	B	325	ARG
1	B	333	GLN
1	B	336	ASN
1	B	366	ARG
1	B	375	GLU
1	B	376	ARG
1	B	380	ASN
1	B	381	THR
1	B	391	GLN
1	B	447	PHE
1	B	448	THR

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Mol	Chain	Res	Type
1	C	18	ILE
1	C	28	GLU
1	C	35	ARG
1	C	40	LEU
1	C	45	SER
1	C	56	ASN
1	C	65	LEU
1	C	75	LEU
1	C	102	LEU
1	C	121	THR
1	C	127	ASN
1	C	137	THR
1	C	142	GLU
1	C	172	LEU
1	C	174	GLN
1	C	178	THR
1	C	179	THR
1	C	185	ASP
1	C	189	THR
1	C	191	LEU
1	C	230	MSE
1	C	242	VAL
1	C	245	MSE
1	C	280	ASP
1	C	285	MSE
1	C	287	LYS
1	C	294	TYR
1	C	307	ASP
1	C	325	ARG
1	C	333	GLN
1	C	336	ASN
1	C	342	SER
1	C	347	SER
1	C	366	ARG
1	C	375	GLU
1	C	376	ARG
1	C	380	ASN
1	C	381	THR
1	C	391	GLN
1	C	447	PHE
1	C	448	THR
1	D	28	GLU

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Mol	Chain	Res	Type
1	D	38	VAL
1	D	45	SER
1	D	56	ASN
1	D	65	LEU
1	D	75	LEU
1	D	91	ARG
1	D	102	LEU
1	D	121	THR
1	D	127	ASN
1	D	137	THR
1	D	142	GLU
1	D	172	LEU
1	D	174	GLN
1	D	178	THR
1	D	179	THR
1	D	185	ASP
1	D	189	THR
1	D	191	LEU
1	D	230	MSE
1	D	242	VAL
1	D	245	MSE
1	D	280	ASP
1	D	284	SER
1	D	285	MSE
1	D	287	LYS
1	D	294	TYR
1	D	307	ASP
1	D	325	ARG
1	D	333	GLN
1	D	336	ASN
1	D	350	ARG
1	D	367	ARG
1	D	375	GLU
1	D	376	ARG
1	D	380	ASN
1	D	381	THR
1	D	391	GLN
1	D	447	PHE
1	D	448	THR
1	E	21	ASN
1	E	22	PHE
1	E	28	GLU

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Mol	Chain	Res	Type
1	E	34	GLU
1	E	40	LEU
1	E	56	ASN
1	E	65	LEU
1	E	75	LEU
1	E	102	LEU
1	E	121	THR
1	E	127	ASN
1	E	137	THR
1	E	142	GLU
1	E	172	LEU
1	E	174	GLN
1	E	178	THR
1	E	179	THR
1	E	185	ASP
1	E	189	THR
1	E	191	LEU
1	E	230	MSE
1	E	242	VAL
1	E	245	MSE
1	E	280	ASP
1	E	285	MSE
1	E	287	LYS
1	E	294	TYR
1	E	307	ASP
1	E	325	ARG
1	E	333	GLN
1	E	336	ASN
1	E	345	LYS
1	E	350	ARG
1	E	353	LYS
1	E	363	ASN
1	E	364	ASP
1	E	367	ARG
1	E	375	GLU
1	E	376	ARG
1	E	380	ASN
1	E	381	THR
1	E	391	GLN
1	E	447	PHE
1	E	448	THR
1	F	22	PHE

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Mol	Chain	Res	Type
1	F	29	ARG
1	F	35	ARG
1	F	37	THR
1	F	38	VAL
1	F	40	LEU
1	F	56	ASN
1	F	65	LEU
1	F	75	LEU
1	F	102	LEU
1	F	121	THR
1	F	127	ASN
1	F	137	THR
1	F	142	GLU
1	F	172	LEU
1	F	174	GLN
1	F	178	THR
1	F	179	THR
1	F	185	ASP
1	F	189	THR
1	F	191	LEU
1	F	230	MSE
1	F	242	VAL
1	F	245	MSE
1	F	254	ASN
1	F	280	ASP
1	F	284	SER
1	F	285	MSE
1	F	287	LYS
1	F	294	TYR
1	F	307	ASP
1	F	325	ARG
1	F	333	GLN
1	F	336	ASN
1	F	348	LYS
1	F	349	PHE
1	F	375	GLU
1	F	376	ARG
1	F	380	ASN
1	F	381	THR
1	F	391	GLN
1	F	447	PHE
1	F	448	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	127	ASN
1	A	141	ASN
1	A	160	ASN
1	A	174	GLN
1	A	186	GLN
1	A	190	ASN
1	A	254	ASN
1	A	289	ASN
1	A	315	ASN
1	A	333	GLN
1	A	336	ASN
1	A	352	ASN
1	A	363	ASN
1	A	368	ASN
1	A	380	ASN
1	A	391	GLN
1	A	405	GLN
1	A	433	ASN
1	B	21	ASN
1	B	127	ASN
1	B	141	ASN
1	B	160	ASN
1	B	174	GLN
1	B	186	GLN
1	B	190	ASN
1	B	254	ASN
1	B	289	ASN
1	B	315	ASN
1	B	336	ASN
1	B	363	ASN
1	B	368	ASN
1	B	380	ASN
1	B	391	GLN
1	B	405	GLN
1	B	433	ASN
1	C	127	ASN
1	C	141	ASN
1	C	160	ASN
1	C	174	GLN
1	C	186	GLN

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Mol	Chain	Res	Type
1	C	190	ASN
1	C	254	ASN
1	C	289	ASN
1	C	315	ASN
1	C	333	GLN
1	C	336	ASN
1	C	352	ASN
1	C	363	ASN
1	C	368	ASN
1	C	380	ASN
1	C	391	GLN
1	C	405	GLN
1	C	424	ASN
1	C	433	ASN
1	D	127	ASN
1	D	141	ASN
1	D	160	ASN
1	D	174	GLN
1	D	186	GLN
1	D	190	ASN
1	D	254	ASN
1	D	289	ASN
1	D	315	ASN
1	D	336	ASN
1	D	352	ASN
1	D	363	ASN
1	D	368	ASN
1	D	380	ASN
1	D	391	GLN
1	D	405	GLN
1	D	433	ASN
1	E	21	ASN
1	E	127	ASN
1	E	141	ASN
1	E	160	ASN
1	E	174	GLN
1	E	186	GLN
1	E	190	ASN
1	E	254	ASN
1	E	289	ASN
1	E	315	ASN
1	E	333	GLN

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Mol	Chain	Res	Type
1	E	336	ASN
1	E	352	ASN
1	E	363	ASN
1	E	380	ASN
1	E	391	GLN
1	E	405	GLN
1	E	433	ASN
1	F	127	ASN
1	F	141	ASN
1	F	160	ASN
1	F	174	GLN
1	F	186	GLN
1	F	190	ASN
1	F	254	ASN
1	F	289	ASN
1	F	315	ASN
1	F	333	GLN
1	F	336	ASN
1	F	363	ASN
1	F	368	ASN
1	F	380	ASN
1	F	391	GLN
1	F	405	GLN
1	F	424	ASN
1	F	433	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	440/460 (95%)	-0.10	0 100 100	13, 47, 89, 107	0
1	B	435/460 (94%)	-0.05	1 (0%) 93 70	21, 54, 95, 109	0
1	C	438/460 (95%)	-0.06	1 (0%) 93 70	15, 50, 92, 109	0
1	D	434/460 (94%)	0.05	1 (0%) 93 70	18, 56, 95, 110	0
1	E	431/460 (93%)	0.06	0 100 100	25, 58, 98, 111	0
1	F	435/460 (94%)	-0.09	1 (0%) 93 70	17, 52, 92, 109	0
All	All	2613/2760 (94%)	-0.03	4 (0%) 93 70	13, 53, 95, 111	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	128	VAL	2.7
1	B	380	ASN	2.2
1	D	106	VAL	2.2
1	C	129	VAL	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.