



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:49 PM UTC

PDB ID : 3LML / pdb_00003lml
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 X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

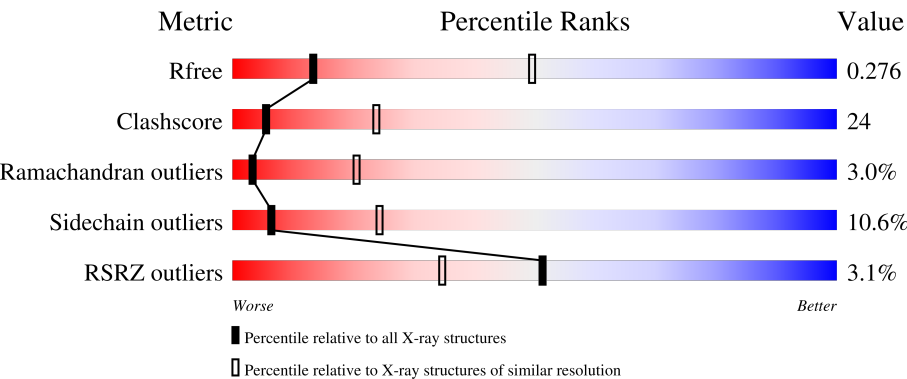
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	460	6% 55% 34% 7% .
1	B	460	% 52% 35% 8% 5%
1	C	460	5% 51% 35% 9% 5%
1	D	460	3% 52% 36% 7% 6%

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Mol	Chain	Length	Quality of chain
1	E	460	% 51%34%9%6%
1	F	460	% 54%34%7%5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20036 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 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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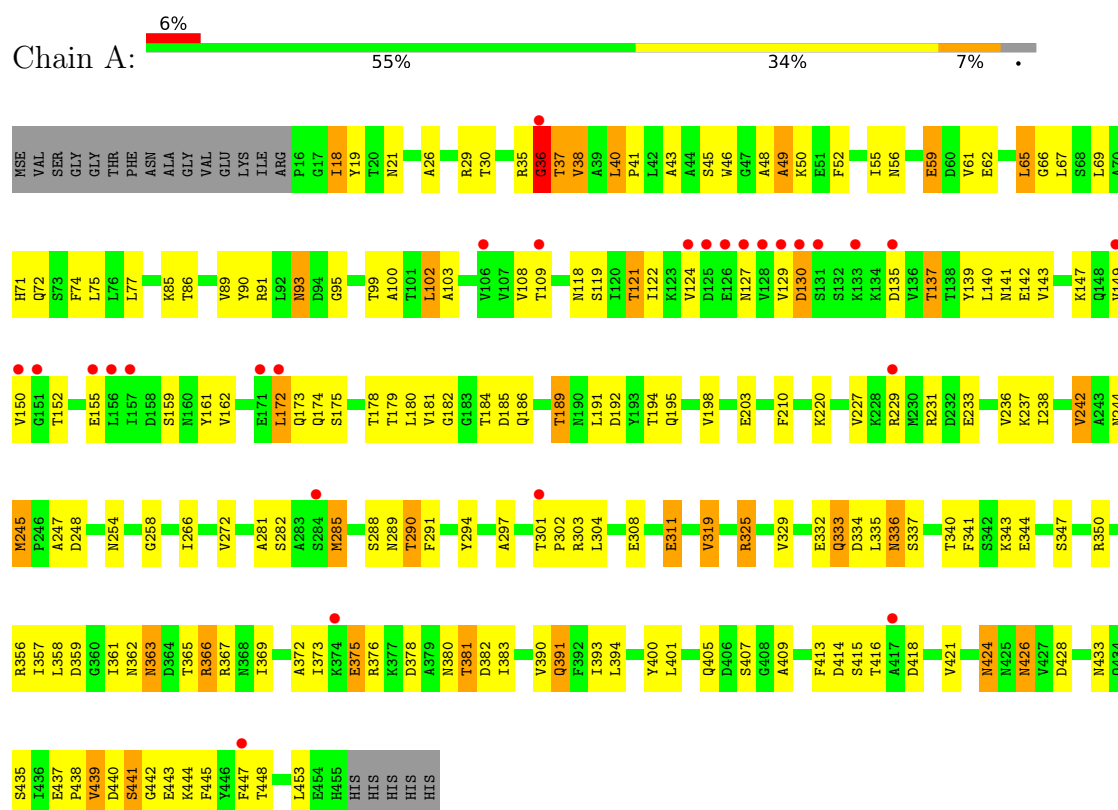
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Chain	Residue	Modelled	Actual	Comment	Reference
C	454	GLU	-	expression tag	UNP Q92CB1
C	455	HIS	-	expression tag	UNP Q92CB1
C	456	HIS	-	expression tag	UNP Q92CB1
C	457	HIS	-	expression tag	UNP Q92CB1
C	458	HIS	-	expression tag	UNP Q92CB1
C	459	HIS	-	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

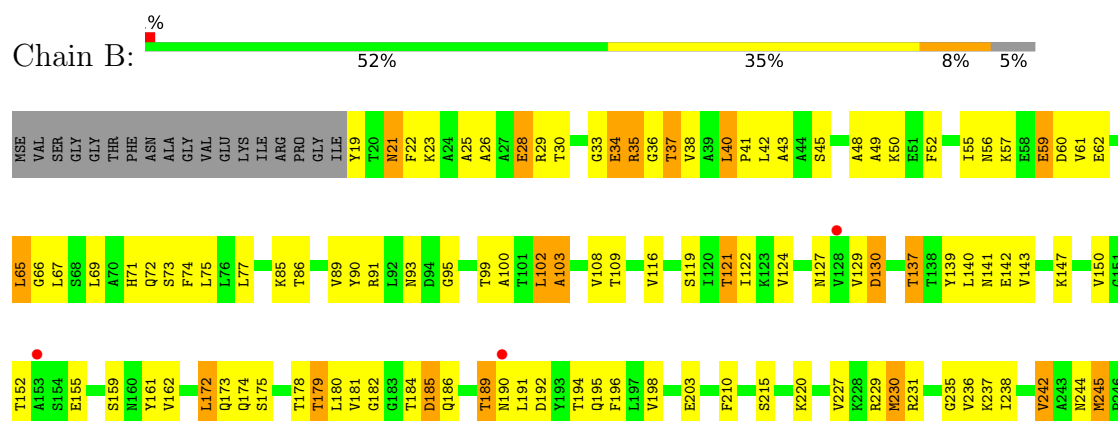
3 Residue-property plots [i](#)

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.

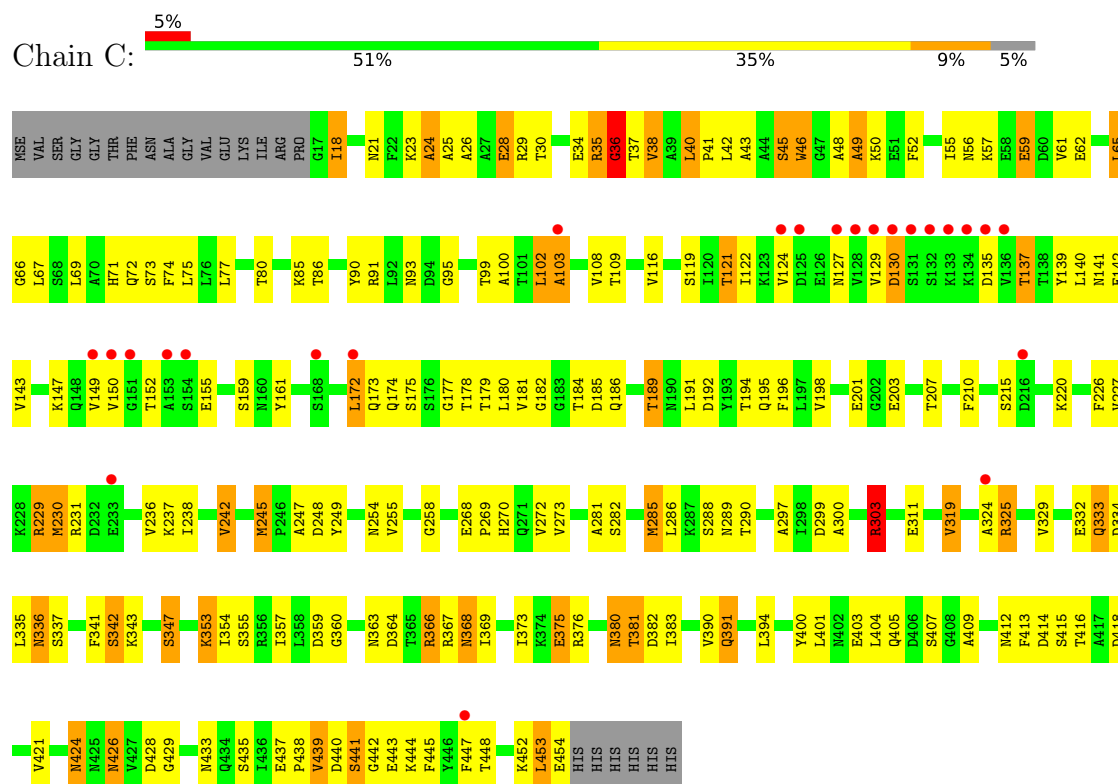
• Molecule 1: Lin1278 protein



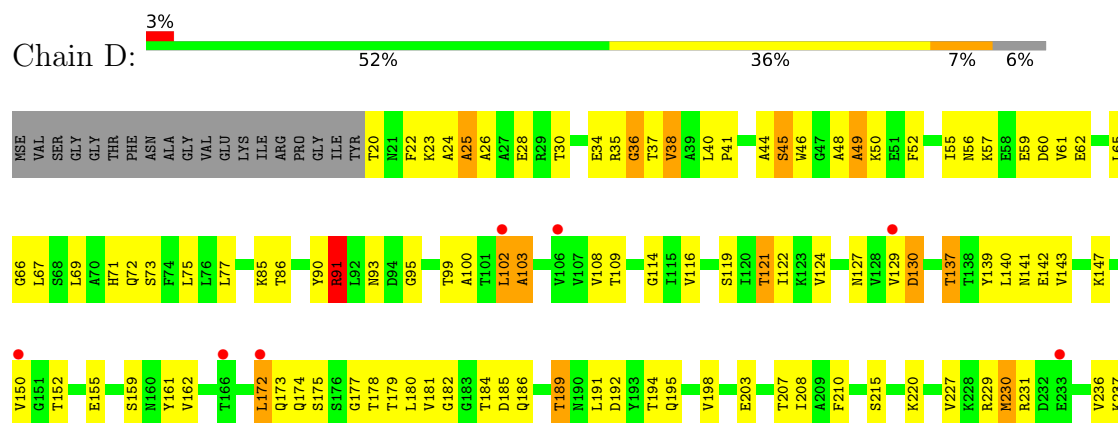
• Molecule 1: Lin1278 protein

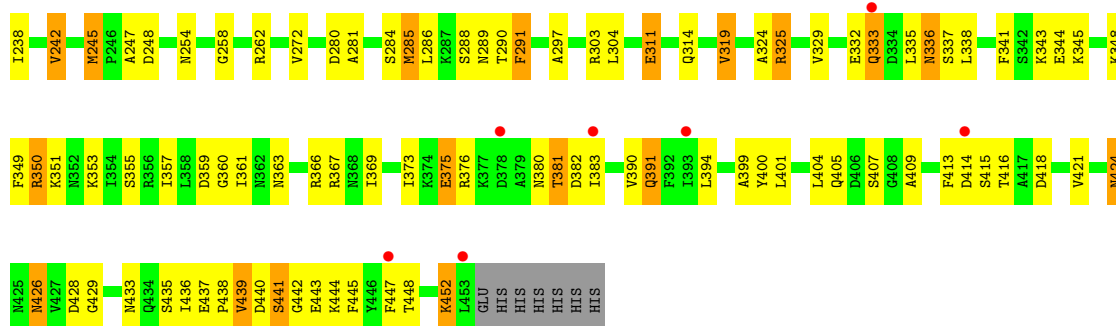


- Molecule 1: Lin1278 protein

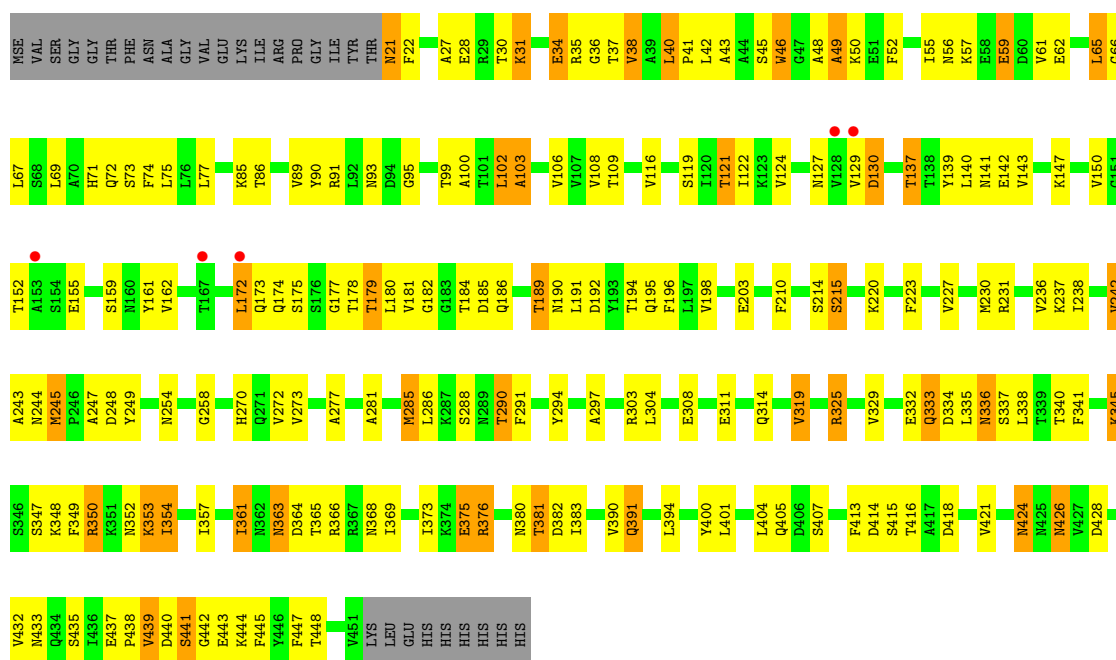


- Molecule 1: Lin1278 protein

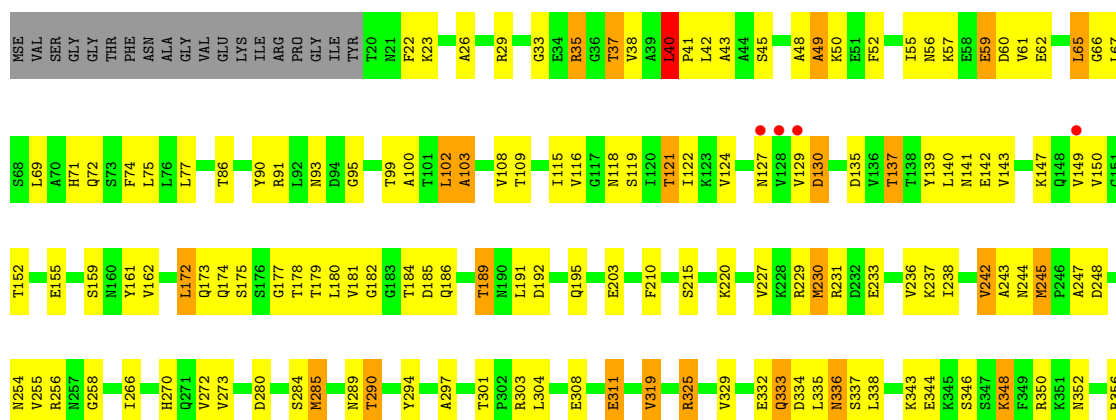




• Molecule 1: Lin1278 protein



• Molecule 1: Lin1278 protein





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 19.96 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.3 (19.96-3.30) 94.6 (19.96-3.30)	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, REFMAC	Depositor
R, R_{free}	0.230 , 0.260 0.249 , 0.276	Depositor DCC
R_{free} test set	4356 reflections (4.91%)	wwPDB-VP
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 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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	0.66	2/3418 (0.1%)	0.93	8/4627 (0.2%)
1	B	0.59	1/3378 (0.0%)	0.90	7/4573 (0.2%)
1	C	0.66	1/3399 (0.0%)	1.00	18/4601 (0.4%)
1	D	0.57	0/3365	1.00	13/4555 (0.3%)
1	E	0.57	1/3341 (0.0%)	0.90	6/4523 (0.1%)
1	F	0.63	1/3374 (0.0%)	0.90	7/4567 (0.2%)
All	All	0.61	6/20275 (0.0%)	0.94	59/27446 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	290	THR	CA-CB	-8.97	1.38	1.53
1	F	290	THR	CA-CB	-8.05	1.39	1.53
1	B	290	THR	C-O	-5.36	1.17	1.24
1	A	290	THR	C-O	-5.27	1.17	1.24
1	A	18	ILE	CA-CB	5.19	1.61	1.54
1	E	290	THR	C-O	-5.13	1.17	1.23

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	ARG	NE-CZ-NH2	12.40	130.36	119.20
1	D	91	ARG	NE-CZ-NH2	-11.96	108.43	119.20
1	C	303	ARG	NE-CZ-NH1	-11.54	109.96	121.50
1	C	229	ARG	NE-CZ-NH2	-11.27	109.06	119.20
1	D	262	ARG	NE-CZ-NH2	-10.66	109.60	119.20
1	D	91	ARG	NE-CZ-NH1	10.16	131.66	121.50
1	C	229	ARG	CD-NE-CZ	10.08	138.52	124.40
1	D	325	ARG	NE-CZ-NH2	-9.43	110.71	119.20
1	D	91	ARG	CD-NE-CZ	9.34	137.48	124.40
1	C	229	ARG	NE-CZ-NH1	9.24	130.74	121.50
1	D	262	ARG	CD-NE-CZ	9.17	137.24	124.40
1	C	325	ARG	NE-CZ-NH2	-8.99	111.11	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	ARG	CD-NE-CZ	8.74	136.63	124.40
1	D	262	ARG	NE-CZ-NH1	8.61	130.11	121.50
1	C	325	ARG	CD-NE-CZ	8.15	135.82	124.40
1	D	325	ARG	CD-NE-CZ	8.10	135.74	124.40
1	D	325	ARG	NE-CZ-NH1	7.42	128.92	121.50
1	C	325	ARG	NE-CZ-NH1	7.28	128.78	121.50
1	D	426	ASN	N-CA-C	-7.25	103.52	112.88
1	E	426	ASN	N-CA-C	-7.17	103.63	112.88
1	C	426	ASN	N-CA-C	-6.85	103.29	112.94
1	D	291	PHE	N-CA-C	-6.75	104.99	113.23
1	F	426	ASN	N-CA-C	-6.58	103.67	112.94
1	B	426	ASN	N-CA-C	-6.57	103.68	112.94
1	A	426	ASN	N-CA-C	-6.54	103.72	112.94
1	C	36	GLY	N-CA-C	6.45	128.47	113.18
1	E	325	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	D	319	VAL	N-CA-C	6.16	117.46	108.53
1	F	325	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	A	325	ARG	NE-CZ-NH1	-6.10	115.40	121.50
1	B	290	THR	CA-C-N	-6.04	114.23	123.47
1	B	290	THR	C-N-CA	-6.04	114.23	123.47
1	B	375	GLU	N-CA-C	-6.00	105.99	113.55
1	E	325	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	A	325	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	B	325	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	B	325	ARG	NE-CZ-NH1	-5.76	115.73	121.50
1	D	375	GLU	N-CA-C	-5.70	106.36	113.55
1	C	375	GLU	N-CA-C	-5.61	106.48	113.55
1	F	375	GLU	N-CA-C	-5.59	106.51	113.55
1	B	319	VAL	N-CA-C	5.54	117.31	108.89
1	F	325	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	C	353	LYS	N-CA-C	-5.49	105.30	111.28
1	A	375	GLU	N-CA-C	-5.39	106.76	113.55
1	F	40	LEU	CA-C-N	5.37	126.55	119.84
1	F	40	LEU	C-N-CA	5.37	126.55	119.84
1	E	375	GLU	N-CA-C	-5.36	106.80	113.55
1	E	361	ILE	CB-CA-C	-5.32	105.06	112.02
1	C	290	THR	OG1-CB-CG2	-5.31	98.67	109.30
1	A	38	VAL	N-CA-C	5.28	116.08	108.48
1	F	319	VAL	N-CA-C	5.21	116.81	108.89
1	A	93	ASN	N-CA-C	5.20	116.69	109.31
1	A	36	GLY	N-CA-C	5.05	125.15	113.18
1	A	319	VAL	N-CA-C	5.04	116.55	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	319	VAL	N-CA-C	5.02	116.53	108.89
1	E	319	VAL	N-CA-C	5.02	116.52	108.89
1	C	368	ASN	N-CA-C	5.02	116.44	111.07
1	C	290	THR	CA-C-N	5.01	129.67	122.40
1	C	290	THR	C-N-CA	5.01	129.67	122.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3376	0	3356	158	0
1	B	3338	0	3321	169	0
1	C	3359	0	3341	173	0
1	D	3326	0	3312	156	0
1	E	3302	0	3281	169	0
1	F	3335	0	3318	150	0
All	All	20036	0	19929	943	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 24.

All (943) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:37:THR:HB	1:A:86:THR:HB	1.54	0.88
1:B:35:ARG:HH12	1:B:284:SER:CA	1.84	0.88
1:E:366:ARG:HH21	1:E:366:ARG:HB2	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:D:229:ARG:HD2	1:F:233:GLU:HB2	1.57	0.85
1:E:30:THR:HG21	1:E:407:SER:HB2	1.58	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:HB2	1:E:366:ARG:NH2	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:B:99:THR:HG22	1:B:100:ALA:H	1.45	0.81
1:D:237:LYS:H	1:D:363:ASN:HD21	1.26	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:B:102:LEU:HD11	1:B:122:ILE:HG21	1.64	0.80
1:D:285:MSE:HE2	1:D:409:ALA:HB1	1.64	0.80
1:E:102:LEU:HD11	1:E:122:ILE:HG21	1.64	0.80
1:E:179:THR:CG2	1:F:181:VAL:HG23	2.11	0.80
1:A:365:THR:O	1:A:369:ILE:HG12	1.82	0.80
1:E:350:ARG:HH21	1:E:350:ARG:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:319:VAL:HG23	1:E:332:GLU:HB2	1.64	0.77
1:F:40:LEU:HD23	1:F:41:PRO:HD2	1.66	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:248:ASP:CG	1:A:340:THR:HG22	2.09	0.77
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.47	0.77
1:F:37:THR:HB	1:F:86:THR:HB	1.67	0.77
1:F:102:LEU:HD11	1:F:122:ILE:HG21	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:A:366:ARG:HB2	1:A:366:ARG:CZ	2.15	0.75
1:E:99:THR:HG23	1:E:109:THR:HG22	1.67	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: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:137:THR:HG22	1:E:147:LYS:HG3	1.72	0.72
1:E:373:ILE:HD13	1:E:383:ILE:HD12	1.70	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:B:405:GLN:HE22	1:B:413:PHE:H	1.34	0.71
1:C:119:SER:HB3	1:C:141:ASN:ND2	2.05	0.71
1:F:356:ARG:HG2	1:F:356:ARG:HH11	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:140:LEU:O	1:D:141:ASN:HB2	1.90	0.70
1:D:338:LEU:HG	1:D:341:PHE:CE1	2.25	0.70
1:E:103:ALA:HB1	1:E:173:GLN:HB2	1.73	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:A:343:LYS:HZ1	1:A:344:GLU:HG3	1.57	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:A:439:VAL:HG23	1:A:440:ASP:H	1.58	0.69
1:B:439:VAL:HG23	1:B:440:ASP:H	1.58	0.69
1:C:137:THR:HG22	1:C:147:LYS:HG3	1.75	0.69
1:C:366:ARG:HB2	1:C:366:ARG:NH2	2.07	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:B:137:THR:HG22	1:B:147:LYS:HG3	1.76	0.68
1:F:352:ASN:O	1:F:356:ARG:HG3	1.94	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
1:E:237:LYS:HB2	1:E:363:ASN:HD21	1.58	0.68
1:B:414:ASP:OD2	1:B:416:THR:HB	1.94	0.68
1:F:37:THR:HA	1:F:86:THR:O	1.93	0.68
1:F:103:ALA:HB1	1:F:173:GLN:HB2	1.74	0.68
1:C:373:ILE:HD13	1:C:383:ILE:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:336:ASN:HD21	1:A:350:ARG:HA	1.60	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: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:C:28:GLU:C	1:C:35:ARG:HH21	2.04	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: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:F:405:GLN:NE2	1:F:413:PHE:H	1.94	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:B:103:ALA:HB1	1:B:173:GLN:H	1.62	0.65
1:E:99:THR:HG22	1:E:100:ALA:N	2.11	0.65
1:A:18:ILE:HD12	1:A:372:ALA:HA	1.79	0.64
1:A:369:ILE:O	1:A:373:ILE:HG12	1.97	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:121:THR:HG23	1:A:139:TYR:HB2	1.80	0.64
1:A:150:VAL:HB	1:A:155:GLU:HB2	1.80	0.64
1:B:150:VAL:HB	1:B:155:GLU:HB2	1.79	0.64
1:C:103:ALA:HB1	1:C:173:GLN:H	1.62	0.64
1:D:373:ILE:HD13	1:D:383:ILE:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ILE:HD12	1:C:18:ILE:H	1.61	0.64
1:D:124:VAL:HG21	1:D:172:LEU:HD22	1.79	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:B:99:THR:HG22	1:B:100:ALA:N	2.12	0.63
1:E:366:ARG:HH21	1:E:366:ARG:CB	2.11	0.63
1:E:414:ASP:OD2	1:E:416:THR:HB	1.98	0.63
1:A:343:LYS:NZ	1:A:344:GLU:HG3	2.13	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: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:F:424:ASN:C	1:F:426:ASN:H	2.07	0.63
1:B:45:SER:OG	1:B:185:ASP:OD2	2.16	0.62
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:C:366:ARG:HH21	1:C:366:ARG:CB	2.12	0.62
1:D:363:ASN:O	1:D:366:ARG:HG2	1.99	0.62
1:D:424:ASN:C	1:D:426:ASN:H	2.08	0.62
1:E:424:ASN:C	1:E:426:ASN:H	2.08	0.62
1:C:150:VAL:HB	1:C:155:GLU:HB2	1.81	0.62
1:C:324:ALA:HB2	1:F:380:ASN:HB2	1.81	0.62
1:D:150:VAL:HB	1:D:155:GLU:HB2	1.80	0.62
1:D:290:THR:O	1:D:291:PHE:HB2	1.99	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:A:258:GLY:HA2	1:A:272:VAL:HG21	1.82	0.61
1:C:285:MSE:HE2	1:C:409:ALA:HB1	1.82	0.61
1:A:414:ASP:OD2	1:A:416:THR:HB	2.00	0.61
1:D:121:THR:HG23	1:D:139:TYR:HB2	1.81	0.61
1:C:99:THR:HG22	1:C:100:ALA:N	2.12	0.61
1:E:121:THR:HG23	1:E:139:TYR:HB2	1.82	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:A:266:ILE:HD11	1:B:190:ASN:N	2.15	0.61
1:A:405:GLN:NE2	1:A:413:PHE:H	1.98	0.61
1:B:424:ASN:C	1:B:426:ASN:H	2.08	0.61
1:E:45:SER:O	1:E:46:TRP:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:MSE:HE1	1:B:404:LEU:HD13	1.82	0.61
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:A:61:VAL:HG21	1:A:69:LEU:HD13	1.82	0.60
1:B:35:ARG:HG3	1:B:36:GLY:N	2.14	0.60
1:B:290:THR:O	1:B:291:PHE:HB2	2.00	0.60
1:F:124:VAL:HG21	1:F:172:LEU:HD22	1.83	0.60
1:B:426:ASN:HB2	1:B:428:ASP:OD1	2.01	0.60
1:C:23:LYS:C	1:C:25:ALA:H	2.09	0.60
1:D:348:LYS:HD2	1:D:348:LYS:N	2.15	0.60
1:A:424:ASN:C	1:A:426:ASN:H	2.10	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:B:121:THR:HG23	1:B:139:TYR:HB2	1.83	0.59
1:C:35:ARG:HB3	1:C:282:SER:HA	1.85	0.59
1:C:424:ASN:C	1:C:426:ASN:H	2.09	0.59
1:C:245:MSE:H	1:C:254:ASN:ND2	2.01	0.59
1:C:354:ILE:N	1:C:354:ILE:HD12	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:A:237:LYS:H	1:A:363:ASN:HD21	1.51	0.58
1:C:324:ALA:CB	1:F:380:ASN:HB2	2.34	0.58
1:C:341:PHE:CD1	1:C:347:SER:HA	2.38	0.58
1:D:414:ASP:OD2	1:D:416:THR:HB	2.03	0.58
1:D:429:GLY:CA	1:D:452:LYS:HA	2.32	0.58
1:A:124:VAL:HG21	1:A:172:LEU:HD22	1.85	0.58
1:B:62:GLU:HA	1:B:67:LEU:O	2.04	0.58
1:B:258:GLY:HA2	1:B:272:VAL:HG21	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LEU:HD11	1:D:122:ILE:CG2	2.33	0.58
1:D:285:MSE:HE1	1:D:404:LEU:HD13	1.85	0.58
1:B:285:MSE:HE2	1:B:409:ALA:HB1	1.86	0.58
1:A:36:GLY:HA3	1:A:281:ALA:O	2.03	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:F:55:ILE:O	1:F:55:ILE:HG13	2.04	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: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:E:341:PHE:CE1	1:E:347:SER:HA	2.39	0.57
1:A:48:ALA:O	1:A:49:ALA:HB3	2.03	0.57
1:A:340:THR:HG23	1:A:340:THR:O	2.05	0.57
1:E:285:MSE:HE1	1:E:361:ILE:HD11	1.87	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:E:102:LEU:HD11	1:E:122:ILE:CG2	2.33	0.56
1:A:18:ILE:O	1:A:21:ASN:HB2	2.05	0.56
1:A:373:ILE:HD12	1:A:453:LEU:HD23	1.85	0.56
1:B:369:ILE:O	1:B:373:ILE:HG12	2.05	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:102:LEU:HD11	1:F:122:ILE:CG2	2.35	0.56
1:F:103:ALA:CB	1:F:173:GLN:H	2.18	0.56
1:E:334:ASP:C	1:E:352:ASN:HD22	2.13	0.56
1:E:48:ALA:O	1:E:49:ALA:HB3	2.05	0.56
1:A:43:ALA:HB1	1:A:93:ASN:ND2	2.20	0.56
1:C:258:GLY:HA2	1:C:272:VAL:HG21	1.87	0.56
1:E:363:ASN:HD22	1:E:363:ASN:N	2.03	0.56
1:F:50:LYS:NZ	1:F:195:GLN:HG3	2.21	0.56
1:A:103:ALA:CB	1:A:173:GLN:H	2.18	0.56
1:A:356:ARG:CG	1:A:356:ARG:NH1	2.65	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: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	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:HG21	1:B:69:LEU:HD13	1.87	0.55
1:C:40:LEU:HD13	1:C:42:LEU:HD11	1.88	0.55
1:D:237:LYS:N	1:D:363:ASN:HD21	2.00	0.55
1:A:290:THR:O	1:A:291:PHE:HB2	2.06	0.55
1:C:29:ARG:HD2	1:C:35:ARG:HH22	1.71	0.55
1:E:179:THR:HG23	1:F:118:ASN:HB3	1.89	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:A:245:MSE:H	1:A:254:ASN:ND2	2.05	0.55
1:C:103:ALA:CB	1:C:173:GLN:H	2.18	0.55
1:F:62:GLU:HA	1:F:67:LEU:O	2.07	0.55
1:A:55:ILE:O	1:A:55:ILE:HG13	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:E:62:GLU:HA	1:E:67:LEU:O	2.07	0.54
1:F:124:VAL:HG13	1:F:175:SER:H	1.72	0.54
1:E:52:PHE:CE1	1:E:90:TYR:HB2	2.41	0.54
1:F:122:ILE:N	1:F:122:ILE:HD12	2.22	0.54
1:D:345:LYS:HA	1:D:349:PHE:CE2	2.43	0.54
1:F:48:ALA:O	1:F:49:ALA:HB3	2.07	0.54
1:C:62:GLU:HA	1:C:67:LEU:O	2.07	0.54
1:A:129:VAL:O	1:A:130:ASP:HB2	2.08	0.54
1:B:248:ASP:HA	1:B:337:SER:O	2.07	0.54
1:C:55:ILE:O	1:C:55:ILE:HG13	2.08	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:C:236:VAL:HG12	1:C:238:ILE:HG23	1.90	0.54
1:D:48:ALA:O	1:D:49:ALA:HB3	2.08	0.54
1:D:91:ARG:HD3	1:D:93:ASN:OD1	2.07	0.54
1:E:50:LYS:NZ	1:E:195:GLN:HG3	2.22	0.54
1:A:290:THR:HG23	1:A:333:GLN:HA	1.90	0.54
1:A:336:ASN:C	1:A:336:ASN:HD22	2.16	0.54
1:C:26:ALA:HB3	1:C:403:GLU:HB3	1.90	0.54
1:C:122:ILE:N	1:C:122:ILE:HD12	2.22	0.54
1:C:61:VAL:HG21	1:C:69:LEU:HD13	1.89	0.53
1:E:345:LYS:HD2	1:E:345:LYS:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:N	1:A:122:ILE:HD12	2.23	0.53
1:E:95:GLY:HA3	1:E:184:THR:O	2.09	0.53
1:F:227:VAL:O	1:F:231:ARG:HG3	2.08	0.53
1:E:122:ILE:N	1:E:122:ILE:HD12	2.23	0.53
1:B:237:LYS:H	1:B:363:ASN:HD21	1.57	0.53
1:B:324:ALA:HB2	1:C:380:ASN:HB2	1.91	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:B:124:VAL:HG13	1:B:175:SER:H	1.72	0.53
1:D:55:ILE:O	1:D:55:ILE:HG13	2.09	0.53
1:D:227:VAL:O	1:D:231:ARG:HG3	2.09	0.53
1:E:391:GLN:NE2	1:E:394:LEU:HD23	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:C:66:GLY:C	1:C:67:LEU:HD22	2.33	0.53
1:D:122:ILE:HD12	1:D:122:ILE:N	2.24	0.53
1:B:122:ILE:HD12	1:B:122:ILE:N	2.25	0.52
1:C:220:LYS:HB3	1:C:245:MSE:HG3	1.91	0.52
1:D:37:THR:CG2	1:D:86:THR:HB	2.39	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:35:ARG:O	1:D:85:LYS:HB3	2.08	0.52
1:D:124:VAL:HG13	1:D:175:SER:H	1.73	0.52
1:C:36:GLY:HA3	1:C:281:ALA:O	2.10	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:F:152:THR:HG22	1:F:155:GLU:HG3	1.92	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:52:PHE:CE1	1:D:90:TYR:HB2	2.44	0.52
1:D:345:LYS:HA	1:D:349:PHE:CD2	2.45	0.52
1:B:19:TYR:C	1:B:21:ASN:H	2.18	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:49:ALA:O	1:E:50:LYS:HB2	2.09	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:E:237:LYS:CB	1:E:363:ASN:HD21	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:435:SER:HA	1:B:445:PHE:O	2.09	0.51
1:E:152:THR:HG22	1:E:155:GLU:HG3	1.92	0.51
1:E:236:VAL:HG12	1:E:238:ILE:HG23	1.92	0.51
1:F:61:VAL:HG21	1:F:69:LEU:HD13	1.91	0.51
1:B:441:SER:O	1:B:443:GLU:N	2.43	0.51
1:E:215:SER:CB	1:F:301:THR:HB	2.37	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:D:34:GLU:HB3	1:D:85:LYS:HD3	1.92	0.51
1:F:152:THR:CG2	1:F:155:GLU:HG3	2.40	0.51
1:D:62:GLU:HA	1:D:67:LEU:O	2.11	0.51
1:A:49:ALA:O	1:A:50:LYS:HB2	2.10	0.51
1:C:38:VAL:HA	1:C:207:THR:O	2.11	0.51
1:D:391:GLN:NE2	1:D:394:LEU:HD23	2.25	0.51
1:E:43:ALA:HB1	1:E:93:ASN:ND2	2.25	0.51
1:F:181:VAL:HG22	1:F:182:GLY:N	2.26	0.51
1:F:424:ASN:HD21	1:F:452:LYS:HZ3	1.58	0.51
1:E:285:MSE:HE1	1:E:404:LEU:HD13	1.93	0.51
1:B:55:ILE:O	1:B:55:ILE:HG13	2.10	0.50
1:C:435:SER:HA	1:C:445:PHE:O	2.11	0.50
1:D:30:THR:HG23	1:D:286:LEU:CG	2.41	0.50
1:F:49:ALA:O	1:F:50:LYS:HB2	2.10	0.50
1:F:50:LYS:HZ3	1:F:195:GLN:HG3	1.73	0.50
1:F:441:SER:O	1:F:443:GLU:N	2.44	0.50
1:A:248:ASP:OD2	1:A:340:THR:CG2	2.57	0.50
1:B:49:ALA:O	1:B:50:LYS:HB2	2.09	0.50
1:B:66:GLY:C	1:B:67:LEU:HD22	2.37	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: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:A:62:GLU:HA	1:A:67:LEU:O	2.12	0.50
1:F:336:ASN:C	1:F:336:ASN:HD22	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:THR:CG2	1:B:155:GLU:HG3	2.41	0.50
1:C:23:LYS:HG2	1:C:403:GLU:HG3	1.92	0.50
1:C:129:VAL:O	1:C:130:ASP:HB2	2.12	0.50
1:E:66:GLY:C	1:E:67:LEU:HD22	2.36	0.50
1:A:152:THR:HG22	1:A:155:GLU:HG3	1.94	0.50
1:B:40:LEU:HD23	1:B:41:PRO:HD2	1.93	0.50
1:C:414:ASP:O	1:C:418:ASP:HB2	2.12	0.50
1:E:336:ASN:C	1:E:336:ASN:HD22	2.19	0.50
1:F:43:ALA:HB1	1:F:93:ASN:ND2	2.26	0.50
1:A:378:ASP:O	1:D:324:ALA:HB1	2.10	0.50
1:D:34:GLU:CB	1:D:85:LYS:HD3	2.42	0.50
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:D:435:SER:HA	1:D:445:PHE:O	2.12	0.50
1:E:414:ASP:O	1:E:418:ASP:HB2	2.12	0.50
1:A:140:LEU:O	1:A:143:VAL:HG12	2.11	0.49
1:B:341:PHE:CZ	1:B:350:ARG:HB2	2.47	0.49
1:C:38:VAL:HG21	1:C:80:THR:HG21	1.94	0.49
1:D:95:GLY:HA3	1:D:184:THR:O	2.12	0.49
1:D:366:ARG:HH21	1:D:366:ARG:HB3	1.76	0.49
1:E:190:ASN:HD21	1:F:266:ILE:HD11	1.76	0.49
1:B:248:ASP:CG	1:B:340:THR:HG22	2.36	0.49
1:C:46:TRP:HB2	1:C:116:VAL:HB	1.93	0.49
1:D:152:THR:HG22	1:D:155:GLU:HG3	1.94	0.49
1:E:179:THR:CB	1:F:181:VAL:HG23	2.42	0.49
1:B:414:ASP:O	1:B:418:ASP:HB2	2.12	0.49
1:E:248:ASP:HA	1:E:337:SER:O	2.13	0.49
1:A:373:ILE:HD12	1:A:453:LEU:CD2	2.42	0.49
1:B:50:LYS:HZ1	1:B:195:GLN:HG3	1.76	0.49
1:B:290:THR:HG23	1:B:333:GLN:HA	1.92	0.49
1:C:95:GLY:HA3	1:C:184:THR:O	2.12	0.49
1:D:23:LYS:C	1:D:25:ALA:H	2.21	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:E:347:SER:C	1:E:349:PHE:H	2.20	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:C:336:ASN:C	1:C:336:ASN:HD22	2.20	0.49
1:A:95:GLY:HA3	1:A:184:THR:O	2.13	0.49
1:B:290:THR:O	1:B:291:PHE:CB	2.58	0.49
1:B:303:ARG:C	1:B:304:LEU:HD12	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:SER:O	1:E:116:VAL:HG23	2.11	0.49
1:E:333:GLN:NE2	1:E:335:LEU:HD21	2.28	0.49
1:B:37:THR:HB	1:B:86:THR:HB	1.95	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:D:336:ASN:C	1:D:336:ASN:HD22	2.20	0.49
1:D:390:VAL:HG13	1:D:421:VAL:HB	1.94	0.49
1:F:189:THR:HG23	1:F:192:ASP:CG	2.38	0.49
1:A:102:LEU:HD12	1:A:108:VAL:HG21	1.95	0.49
1:B:23:LYS:HZ2	1:B:403:GLU:HG2	1.78	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: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:D:220:LYS:HB3	1:D:245:MSE:HG3	1.94	0.48
1:F:356:ARG:HH11	1:F:356:ARG:CG	2.25	0.48
1:A:152:THR:CG2	1:A:155:GLU:HG3	2.43	0.48
1:A:336:ASN:ND2	1:A:350:ARG:HA	2.27	0.48
1:A:414:ASP:C	1:A:416:THR:N	2.71	0.48
1:B:124:VAL:HG13	1:B:175:SER:N	2.28	0.48
1:B:336:ASN:C	1:B:336:ASN:HD22	2.22	0.48
1:D:124:VAL:HG13	1:D:175:SER:N	2.28	0.48
1:D:360:GLY:O	1:D:361:ILE:C	2.55	0.48
1:A:220:LYS:HB3	1:A:245:MSE:HG3	1.94	0.48
1:A:414:ASP:O	1:A:418:ASP:HB2	2.13	0.48
1:B:25:ALA:HA	1:B:28:GLU:HG2	1.96	0.48
1:E:369:ILE:HD12	1:E:369:ILE:N	2.29	0.48
1:F:391:GLN:NE2	1:F:394:LEU:HD23	2.27	0.48
1:B:52:PHE:CE1	1:B:90:TYR:HB2	2.48	0.48
1:C:30:THR:HB	1:C:286:LEU:CD1	2.41	0.48
1:A:127:ASN:HB3	1:A:130:ASP:O	2.14	0.48
1:A:181:VAL:HG22	1:A:182:GLY:N	2.28	0.48
1:B:129:VAL:O	1:B:130:ASP:HB2	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:F:129:VAL:O	1:F:129:VAL:HG12	2.13	0.48
1:A:66:GLY:C	1:A:67:LEU:HD22	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:HIS:O	1:E:273:VAL:HG22	2.14	0.48
1:A:438:PRO:O	1:A:439:VAL:C	2.56	0.48
1:D:152:THR:CG2	1:D:155:GLU:HG3	2.43	0.48
1:D:366:ARG:HB3	1:D:366:ARG:NH2	2.29	0.48
1:B:227:VAL:O	1:B:231:ARG:HG3	2.13	0.48
1:E:37:THR:HA	1:E:86:THR:O	2.14	0.48
1:F:435:SER:HA	1:F:445:PHE:O	2.14	0.48
1:D:66:GLY:C	1:D:67:LEU:HD22	2.39	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:A:435:SER:HA	1:A:445:PHE:O	2.14	0.47
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:F:454:GLU:O	1:F:454:GLU:HG3	2.14	0.47
1:A:414:ASP:C	1:A:416:THR:H	2.22	0.47
1:B:220:LYS:HB3	1:B:245:MSE:HG3	1.95	0.47
1:B:354:ILE:H	1:B:354:ILE:HD12	1.79	0.47
1:C:229:ARG:O	1:C:230:MSE:C	2.57	0.47
1:C:414:ASP:C	1:C:416:THR:N	2.72	0.47
1:D:237:LYS:HB3	1:D:359:ASP:OD2	2.14	0.47
1:B:95:GLY:HA3	1:B:184:THR:O	2.14	0.47
1:E:49:ALA:HA	1:E:91:ARG:HD3	1.96	0.47
1:E:50:LYS:HZ3	1:E:195:GLN:HG3	1.80	0.47
1:F:102:LEU:HD12	1:F:108:VAL:HG21	1.95	0.47
1:F:348:LYS:H	1:F:348:LYS:HD2	1.80	0.47
1:B:102:LEU:HD12	1:B:108:VAL:HG21	1.97	0.47
1:C:35:ARG:CG	1:C:35:ARG:HH11	2.26	0.47
1:E:34:GLU:O	1:E:35:ARG:HG3	2.14	0.47
1:A:52:PHE:CE1	1:A:90:TYR:HB2	2.49	0.47
1:D:52:PHE:CD2	1:D:203:GLU:HG3	2.48	0.47
1:A:266:ILE:HD13	1:B:190:ASN:ND2	2.28	0.47
1:B:140:LEU:O	1:B:143:VAL:HG12	2.14	0.47
1:B:391:GLN:NE2	1:B:394:LEU:HD23	2.28	0.47
1:C:57:LYS:HB3	1:C:59:GLU:OE2	2.15	0.47
1:D:438:PRO:O	1:D:439:VAL:C	2.57	0.47
1:E:30:THR:HG23	1:E:286:LEU:CD1	2.35	0.47
1:F:45:SER:HB3	1:F:115:ILE:HG12	1.97	0.47
1:F:390:VAL:HG13	1:F:421:VAL:HB	1.95	0.47
1:F:414:ASP:O	1:F:418:ASP:HB2	2.14	0.47
1:A:40:LEU:O	1:A:89:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ALA:HB3	1:A:329:VAL:CG1	2.44	0.47
1:A:391:GLN:NE2	1:A:394:LEU:HD23	2.30	0.47
1:B:33:GLY:O	1:B:34:GLU:C	2.58	0.47
1:B:65:LEU:HD23	1:B:74:PHE:CE2	2.50	0.47
1:B:341:PHE:HZ	1:B:350:ARG:HB2	1.79	0.47
1:B:438:PRO:O	1:B:439:VAL:C	2.58	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: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:A:285:MSE:CE	1:A:357:ILE:HG23	2.31	0.47
1:C:52:PHE:CE1	1:C:90:TYR:HB2	2.50	0.47
1:E:333:GLN:CD	1:E:335:LEU:HD21	2.38	0.47
1:F:52:PHE:CD2	1:F:203:GLU:HG3	2.50	0.47
1:A:333:GLN:NE2	1:A:335:LEU:HD21	2.30	0.47
1:C:181:VAL:HG22	1:C:182:GLY:N	2.30	0.47
1:C:438:PRO:O	1:C:439:VAL:C	2.58	0.47
1:E:353:LYS:O	1:E:357:ILE:HD11	2.14	0.47
1:F:23:LYS:HG2	1:F:403:GLU:CG	2.45	0.47
1:F:334:ASP:OD2	1:F:352:ASN:HB2	2.15	0.47
1:F:414:ASP:C	1:F:416:THR:N	2.71	0.47
1:A:233:GLU:OE2	1:C:226:PHE:HA	2.15	0.47
1:A:236:VAL:HG12	1:A:238:ILE:HG23	1.97	0.47
1:A:358:LEU:O	1:A:359:ASP:C	2.56	0.47
1:E:354:ILE:O	1:E:357:ILE:HG12	2.15	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:F:333:GLN:CD	1:F:335:LEU:HD21	2.40	0.46
1:A:35:ARG:HB3	1:A:282:SER:HA	1.97	0.46
1:A:124:VAL:HG13	1:A:175:SER:N	2.30	0.46
1:B:235:GLY:C	1:B:366:ARG:HH12	2.22	0.46
1:C:23:LYS:C	1:C:25:ALA:N	2.72	0.46
1:C:424:ASN:HD21	1:C:452:LYS:NZ	2.12	0.46
1:D:50:LYS:HZ1	1:D:195:GLN:HG3	1.78	0.46
1:D:441:SER:O	1:D:443:GLU:N	2.46	0.46
1:F:66:GLY:C	1:F:67:LEU:HD22	2.40	0.46
1:F:140:LEU:O	1:F:143:VAL:HG12	2.15	0.46
1:F:356:ARG:HG2	1:F:356:ARG:NH1	2.28	0.46
1:F:438:PRO:O	1:F:439:VAL:C	2.58	0.46
1:A:181:VAL:HG23	1:B:179:THR:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:O	1:A:382:ASP:C	2.59	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:35:ARG:CG	1:C:35:ARG:NH1	2.78	0.46
1:C:100:ALA:HB2	1:C:180:LEU:HA	1.96	0.46
1:C:441:SER:O	1:C:443:GLU:N	2.48	0.46
1:D:20:THR:C	1:D:24:ALA:HB2	2.41	0.46
1:A:266:ILE:HD11	1:B:190:ASN:CG	2.41	0.46
1:A:333:GLN:CD	1:A:335:LEU:HD21	2.41	0.46
1:A:369:ILE:HD12	1:A:393:ILE:HG23	1.98	0.46
1:D:41:PRO:O	1:D:41:PRO:HG2	2.15	0.46
1:D:129:VAL:O	1:D:129:VAL:HG12	2.16	0.46
1:E:180:LEU:HD12	1:E:180:LEU:N	2.31	0.46
1:E:441:SER:O	1:E:443:GLU:N	2.49	0.46
1:A:71:HIS:ND1	1:A:72:GLN:N	2.64	0.46
1:C:333:GLN:NE2	1:C:335:LEU:HD21	2.31	0.46
1:D:46:TRP:HB2	1:D:116:VAL:HB	1.98	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:A:390:VAL:HG13	1:A:421:VAL:HB	1.98	0.46
1:C:390:VAL:HG13	1:C:421:VAL:HB	1.97	0.46
1:E:55:ILE:O	1:E:55:ILE:HG13	2.14	0.46
1:E:71:HIS:CE1	1:E:73:SER:HG	2.34	0.46
1:E:214:SER:HA	1:E:220:LYS:NZ	2.30	0.46
1:F:414:ASP:C	1:F:416:THR:H	2.24	0.46
1:A:180:LEU:N	1:A:180:LEU:HD12	2.30	0.46
1:A:210:PHE:HB3	1:A:242:VAL:CG1	2.46	0.46
1:B:52:PHE:CD2	1:B:203:GLU:HG3	2.50	0.46
1:B:229:ARG:O	1:B:230:MSE:C	2.59	0.46
1:B:288:SER:OG	1:B:289:ASN:N	2.48	0.46
1:C:140:LEU:O	1:C:143:VAL:HG12	2.16	0.46
1:E:438:PRO:O	1:E:439:VAL:C	2.58	0.46
1:C:124:VAL:HG13	1:C:175:SER:N	2.30	0.46
1:D:23:LYS:HE2	1:D:399:ALA:HB1	1.98	0.46
1:D:127:ASN:HB3	1:D:130:ASP:O	2.15	0.46
1:E:181:VAL:HG22	1:E:182:GLY:N	2.31	0.46
1:B:362:ASN:HB2	1:B:447:PHE:CD2	2.51	0.45
1:B:414:ASP:C	1:B:416:THR:N	2.71	0.45
1:C:237:LYS:H	1:C:363:ASN:HD21	1.64	0.45
1:E:102:LEU:HD12	1:E:108:VAL:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:THR:HG23	1:B:192:ASP:CG	2.42	0.45
1:C:414:ASP:C	1:C:416:THR:H	2.24	0.45
1:D:297:ALA:HB3	1:D:329:VAL:CG1	2.46	0.45
1:E:414:ASP:C	1:E:416:THR:N	2.73	0.45
1:F:71:HIS:ND1	1:F:72:GLN:N	2.64	0.45
1:A:189:THR:HG23	1:A:192:ASP:CG	2.41	0.45
1:B:34:GLU:HB3	1:B:85:LYS:HD3	1.99	0.45
1:B:45:SER:O	1:B:116:VAL:HG23	2.17	0.45
1:B:390:VAL:HG13	1:B:421:VAL:HB	1.98	0.45
1:C:189:THR:HG23	1:C:192:ASP:CG	2.41	0.45
1:C:288:SER:OG	1:C:289:ASN:N	2.49	0.45
1:E:129:VAL:O	1:E:129:VAL:HG12	2.17	0.45
1:B:341:PHE:CD1	1:B:347:SER:HA	2.52	0.45
1:C:103:ALA:HB2	1:C:173:GLN:O	2.17	0.45
1:D:361:ILE:CD1	1:D:436:ILE:HG21	2.47	0.45
1:D:367:ARG:HG2	1:D:367:ARG:HH21	1.81	0.45
1:E:189:THR:HG23	1:E:192:ASP:CG	2.42	0.45
1:F:297:ALA:HB3	1:F:329:VAL:CG1	2.46	0.45
1:A:414:ASP:O	1:A:416:THR:N	2.49	0.45
1:A:441:SER:O	1:A:443:GLU:N	2.50	0.45
1:B:180:LEU:HD12	1:B:180:LEU:N	2.31	0.45
1:C:29:ARG:HA	1:C:35:ARG:CZ	2.45	0.45
1:C:71:HIS:CE1	1:C:73:SER:HG	2.35	0.45
1:C:288:SER:HB2	1:C:353:LYS:HD2	1.97	0.45
1:A:247:ALA:O	1:A:248:ASP:C	2.59	0.45
1:A:366:ARG:HG3	1:A:367:ARG:N	2.32	0.45
1:C:129:VAL:O	1:C:129:VAL:HG12	2.16	0.45
1:D:100:ALA:HB2	1:D:180:LEU:HA	1.98	0.45
1:E:297:ALA:HB3	1:E:329:VAL:CG1	2.46	0.45
1:F:180:LEU:N	1:F:180:LEU:HD12	2.31	0.45
1:F:369:ILE:HD12	1:F:393:ILE:HG23	1.98	0.45
1:A:122:ILE:HD11	1:A:162:VAL:HG11	1.99	0.45
1:B:210:PHE:HB3	1:B:242:VAL:CG1	2.47	0.45
1:D:44:ALA:HB3	1:D:91:ARG:CG	2.41	0.45
1:A:361:ILE:HG22	1:A:362:ASN:N	2.31	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:HG23	1:E:340:THR:O	2.17	0.45
1:E:414:ASP:C	1:E:416:THR:H	2.25	0.45
1:F:359:ASP:O	1:F:360:GLY:C	2.60	0.45
1:F:381:THR:O	1:F:382:ASP:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:HIS:ND1	1:B:72:GLN:N	2.65	0.45
1:E:127:ASN:HB3	1:E:130:ASP:O	2.16	0.45
1:F:100:ALA:HB2	1:F:180:LEU:HA	1.98	0.45
1:F:289:ASN:HD22	1:F:289:ASN:HA	1.55	0.45
1:B:311:GLU:O	1:B:314:GLN:HB3	2.17	0.44
1:C:18:ILE:HD12	1:C:18:ILE:N	2.30	0.44
1:E:303:ARG:C	1:E:304:LEU:HD12	2.41	0.44
1:F:65:LEU:HD23	1:F:74:PHE:CE2	2.52	0.44
1:F:135:ASP:OD2	1:F:149:VAL:HG22	2.17	0.44
1:F:424:ASN:C	1:F:426:ASN:N	2.75	0.44
1:A:29:ARG:HD2	1:A:285:MSE:SE	2.66	0.44
1:B:129:VAL:O	1:B:129:VAL:HG12	2.16	0.44
1:B:297:ALA:HB3	1:B:329:VAL:CG1	2.47	0.44
1:B:437:GLU:HB2	1:B:444:LYS:HG2	1.98	0.44
1:C:38:VAL:HG21	1:C:80:THR:CG2	2.47	0.44
1:C:71:HIS:ND1	1:C:72:GLN:N	2.65	0.44
1:D:71:HIS:ND1	1:D:72:GLN:N	2.65	0.44
1:E:57:LYS:HB3	1:E:59:GLU:OE2	2.17	0.44
1:E:311:GLU:O	1:E:314:GLN:HB3	2.18	0.44
1:B:122:ILE:HD11	1:B:162:VAL:HG11	1.99	0.44
1:B:333:GLN:NE2	1:B:335:LEU:HD21	2.32	0.44
1:C:29:ARG:CA	1:C:35:ARG:NH2	2.80	0.44
1:C:359:ASP:O	1:C:360:GLY:C	2.59	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:E:124:VAL:HG13	1:E:175:SER:N	2.32	0.44
1:E:288:SER:HB2	1:E:353:LYS:HG2	1.99	0.44
1:D:36:GLY:HA3	1:D:281:ALA:O	2.16	0.44
1:D:140:LEU:O	1:D:143:VAL:HG12	2.17	0.44
1:A:29:ARG:HB3	1:A:285:MSE:SE	2.68	0.44
1:B:49:ALA:HA	1:B:91:ARG:HD3	2.00	0.44
1:C:373:ILE:HD12	1:C:453:LEU:HD12	1.98	0.44
1:D:414:ASP:C	1:D:416:THR:N	2.74	0.44
1:A:100:ALA:HB2	1:A:180:LEU:HA	1.99	0.44
1:A:288:SER:OG	1:A:289:ASN:N	2.51	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:D:351:LYS:NZ	1:D:353:LYS:HB3	2.32	0.44
1:B:433:ASN:N	1:B:433:ASN:HD22	2.14	0.44
1:C:245:MSE:H	1:C:254:ASN:HD21	1.65	0.44
1:D:247:ALA:O	1:D:248:ASP:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:343:LYS:HG3	1:F:344:GLU:N	2.33	0.44
1:A:26:ALA:HB2	1:A:400:TYR:CD1	2.53	0.44
1:A:433:ASN:N	1:A:433:ASN:HD22	2.15	0.44
1:B:42:LEU:HD12	1:B:89:VAL:HG23	1.99	0.44
1:B:247:ALA:O	1:B:248:ASP:C	2.58	0.44
1:C:194:THR:O	1:C:198:VAL:HG23	2.18	0.44
1:C:333:GLN:CD	1:C:335:LEU:HD21	2.42	0.44
1:E:71:HIS:ND1	1:E:72:GLN:N	2.66	0.44
1:E:381:THR:O	1:E:382:ASP:C	2.61	0.44
1:F:127:ASN:HB3	1:F:130:ASP:O	2.18	0.44
1:B:333:GLN:CD	1:B:335:LEU:HD21	2.43	0.43
1:D:71:HIS:CE1	1:D:73:SER:HG	2.35	0.43
1:E:285:MSE:HE3	1:E:357:ILE:HG23	2.00	0.43
1:B:127:ASN:HB3	1:B:130:ASP:O	2.18	0.43
1:C:50:LYS:HZ1	1:C:195:GLN:HG3	1.82	0.43
1:C:354:ILE:N	1:C:354:ILE:CD1	2.80	0.43
1:C:452:LYS:O	1:C:454:GLU:N	2.50	0.43
1:C:270:HIS:O	1:C:273:VAL:HG22	2.18	0.43
1:D:180:LEU:N	1:D:180:LEU:HD12	2.33	0.43
1:D:285:MSE:HG2	1:D:357:ILE:CG1	2.39	0.43
1:D:400:TYR:HD2	1:D:401:LEU:HD22	1.83	0.43
1:E:99:THR:CG2	1:E:100:ALA:H	2.21	0.43
1:E:400:TYR:HD2	1:E:401:LEU:HD22	1.84	0.43
1:B:41:PRO:HB3	1:B:196:PHE:CD1	2.53	0.43
1:B:45:SER:HG	1:B:185:ASP:CG	2.23	0.43
1:C:41:PRO:O	1:C:41:PRO:HG2	2.19	0.43
1:C:135:ASP:OD2	1:C:149:VAL:HG22	2.17	0.43
1:D:424:ASN:C	1:D:426:ASN:N	2.76	0.43
1:F:57:LYS:HB3	1:F:59:GLU:OE2	2.17	0.43
1:F:270:HIS:O	1:F:273:VAL:HG22	2.18	0.43
1:B:414:ASP:C	1:B:416:THR:H	2.25	0.43
1:D:189:THR:HG23	1:D:192:ASP:CG	2.44	0.43
1:E:65:LEU:HD23	1:E:74:PHE:CE2	2.52	0.43
1:F:159:SER:C	1:F:161:TYR:H	2.25	0.43
1:A:43:ALA:HB1	1:A:93:ASN:HD22	1.82	0.43
1:A:159:SER:C	1:A:161:TYR:H	2.25	0.43
1:B:100:ALA:HB2	1:B:180:LEU:HA	2.00	0.43
1:C:99:THR:CG2	1:C:100:ALA:N	2.82	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:D:290:THR:O	1:D:291:PHE:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:LYS:HD3	1:E:245:MSE:HG2	2.01	0.43
1:F:42:LEU:HD23	1:F:42:LEU:HA	1.77	0.43
1:A:45:SER:O	1:A:46:TRP:HB2	2.17	0.43
1:A:229:ARG:HD2	1:C:201:GLU:OE1	2.19	0.43
1:C:268:GLU:O	1:C:269:PRO:C	2.61	0.43
1:E:433:ASN:N	1:E:433:ASN:HD22	2.16	0.43
1:F:414:ASP:O	1:F:416:THR:N	2.50	0.43
1:B:159:SER:C	1:B:161:TYR:H	2.27	0.43
1:B:181:VAL:HG22	1:B:182:GLY:N	2.34	0.43
1:D:122:ILE:HD11	1:D:162:VAL:HG11	2.01	0.43
1:F:220:LYS:HB3	1:F:245:MSE:HG3	2.00	0.43
1:F:247:ALA:O	1:F:248:ASP:C	2.60	0.43
1:B:220:LYS:HD3	1:B:245:MSE:HG2	2.01	0.43
1:B:237:LYS:HB3	1:B:359:ASP:CG	2.43	0.43
1:E:103:ALA:HB1	1:E:173:GLN:N	2.31	0.43
1:E:376:ARG:HD2	1:E:376:ARG:HA	1.80	0.43
1:F:229:ARG:O	1:F:230:MSE:C	2.62	0.43
1:A:400:TYR:HD2	1:A:401:LEU:HD22	1.84	0.43
1:C:49:ALA:HA	1:C:91:ARG:HD3	2.01	0.43
1:D:22:PHE:C	1:D:24:ALA:H	2.27	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:A:30:THR:HG21	1:A:407:SER:OG	2.18	0.42
1:A:35:ARG:O	1:A:36:GLY:O	2.37	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:E:319:VAL:HG23	1:E:332:GLU:CB	2.44	0.42
1:A:308:GLU:O	1:A:311:GLU:HB3	2.19	0.42
1:C:289:ASN:HB2	1:C:334:ASP:CG	2.43	0.42
1:C:381:THR:O	1:C:382:ASP:C	2.62	0.42
1:D:30:THR:HG23	1:D:286:LEU:CD1	2.49	0.42
1:D:333:GLN:CD	1:D:335:LEU:HD21	2.43	0.42
1:E:21:ASN:HD22	1:E:22:PHE:H	1.62	0.42
1:E:345:LYS:HB2	1:E:349:PHE:CD2	2.54	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:B:381:THR:O	1:B:382:ASP:C	2.61	0.42
1:C:180:LEU:N	1:C:180:LEU:HD12	2.35	0.42
1:C:354:ILE:O	1:C:355:SER:C	2.62	0.42
1:A:65:LEU:HD23	1:A:74:PHE:CE2	2.55	0.42
1:A:99:THR:O	1:A:100:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ARG:HG2	1:C:36:GLY:H	1.84	0.42
1:D:335:LEU:HD22	1:D:350:ARG:HD3	2.01	0.42
1:B:103:ALA:HB2	1:B:173:GLN:O	2.20	0.42
1:C:21:ASN:HA	1:C:24:ALA:HB3	2.01	0.42
1:C:255:VAL:HG21	1:C:273:VAL:HG12	2.01	0.42
1:C:437:GLU:HB2	1:C:444:LYS:HG2	2.01	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:E:247:ALA:O	1:E:248:ASP:C	2.62	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:F:243:ALA:HB2	1:F:270:HIS:HA	2.02	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:E:159:SER:C	1:E:161:TYR:H	2.26	0.42
1:E:308:GLU:O	1:E:311:GLU:HB3	2.19	0.42
1:F:433:ASN:N	1:F:433:ASN:HD22	2.17	0.42
1:A:437:GLU:HB2	1:A:444:LYS:HG2	2.02	0.42
1:B:336:ASN:ND2	1:B:338:LEU:HB3	2.35	0.42
1:C:400:TYR:HD2	1:C:401:LEU:HD22	1.85	0.42
1:C:414:ASP:O	1:C:416:THR:N	2.52	0.42
1:D:366:ARG:CG	1:D:367:ARG:N	2.82	0.42
1:E:103:ALA:HB2	1:E:173:GLN:O	2.20	0.42
1:E:369:ILE:HD12	1:E:369:ILE:H	1.85	0.42
1:F:57:LYS:O	1:F:60:ASP:HB2	2.20	0.42
1:F:99:THR:O	1:F:100:ALA:HB2	2.20	0.42
1:F:102:LEU:HD23	1:F:103:ALA:H	1.85	0.42
1:B:103:ALA:HB1	1:B:173:GLN:CB	2.46	0.42
1:C:26:ALA:CB	1:C:403:GLU:HB3	2.49	0.42
1:C:45:SER:O	1:C:46:TRP:HB2	2.19	0.42
1:D:159:SER:C	1:D:161:TYR:H	2.27	0.42
1:D:207:THR:HG22	1:D:208:ILE:N	2.35	0.42
1:D:285:MSE:HE2	1:D:409:ALA:CB	2.44	0.42
1:D:369:ILE:O	1:D:373:ILE:HG12	2.19	0.42
1:E:336:ASN:ND2	1:E:350:ARG:HA	2.30	0.42
1:E:437:GLU:HB2	1:E:444:LYS:HG2	2.02	0.42
1:F:122:ILE:HD11	1:F:162:VAL:HG11	2.02	0.42
1:A:18:ILE:O	1:A:21:ASN:N	2.50	0.42
1:A:119:SER:HB3	1:A:141:ASN:HD21	1.84	0.42
1:B:30:THR:HG21	1:B:407:SER:OG	2.19	0.42
1:D:210:PHE:HB3	1:D:242:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:THR:O	1:D:382:ASP:C	2.63	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: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:F:437:GLU:HB2	1:F:444:LYS:HG2	2.02	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:C:30:THR:HG21	1:C:407:SER:OG	2.18	0.42
1:D:433:ASN:N	1:D:433:ASN:HD22	2.15	0.42
1:E:122:ILE:HD11	1:E:162:VAL:HG11	2.02	0.42
1:A:52:PHE:CD2	1:A:203:GLU:HG3	2.54	0.41
1:A:245:MSE:H	1:A:254:ASN:HD21	1.67	0.41
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:C:65:LEU:HD23	1:C:74:PHE:CE2	2.55	0.41
1:D:229:ARG:O	1:D:230:MSE:C	2.61	0.41
1:E:194:THR:O	1:E:198:VAL:HG23	2.20	0.41
1:E:432:VAL:C	1:E:433:ASN:HD22	2.28	0.41
1:A:194:THR:O	1:A:198:VAL:HG23	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:D:355:SER:O	1:D:359:ASP:HB2	2.20	0.41
1:A:285:MSE:O	1:A:357:ILE:HD11	2.20	0.41
1:C:247:ALA:O	1:C:248:ASP:C	2.62	0.41
1:F:255:VAL:HG21	1:F:273:VAL:HG12	2.01	0.41
1:A:301:THR:HA	1:A:302:PRO:HA	1.92	0.41
1:A:424:ASN:C	1:A:426:ASN:N	2.78	0.41
1:B:102:LEU:HD23	1:B:103:ALA:H	1.85	0.41
1:B:273:VAL:HG23	1:B:274:ALA:N	2.35	0.41
1:C:37:THR:HG22	1:C:86:THR:HB	2.03	0.41
1:C:119:SER:HB3	1:C:141:ASN:HD21	1.82	0.41
1:C:159:SER:C	1:C:161:TYR:H	2.27	0.41
1:D:22:PHE:C	1:D:24:ALA:N	2.76	0.41
1:E:36:GLY:HA3	1:E:281:ALA:O	2.20	0.41
1:E:59:GLU:H	1:E:59:GLU:CD	2.28	0.41
1:E:294:TYR:HB3	1:E:329:VAL:HG13	2.03	0.41
1:A:26:ALA:O	1:A:29:ARG:HB2	2.20	0.41
1:A:50:LYS:HZ1	1:A:195:GLN:HG3	1.85	0.41
1:B:57:LYS:HB3	1:B:59:GLU:OE2	2.20	0.41
1:B:71:HIS:CE1	1:B:73:SER:HG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLU:HB3	1:C:85:LYS:HB2	2.02	0.41
1:C:38:VAL:HG12	1:C:281:ALA:HB2	2.03	0.41
1:C:364:ASP:O	1:C:368:ASN:HB2	2.21	0.41
1:D:414:ASP:C	1:D:416:THR:H	2.28	0.41
1:F:256:ARG:HB3	1:F:319:VAL:HG12	2.01	0.41
1:A:303:ARG:C	1:A:304:LEU:HD12	2.46	0.41
1:B:26:ALA:HB1	1:B:403:GLU:HB3	2.02	0.41
1:B:102:LEU:O	1:B:103:ALA:C	2.63	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:D:245:MSE:H	1:D:254:ASN:HD21	1.68	0.41
1:E:99:THR:O	1:E:100:ALA:HB2	2.21	0.41
1:E:100:ALA:HB2	1:E:180:LEU:HA	2.03	0.41
1:B:354:ILE:HD12	1:B:354:ILE:N	2.35	0.41
1:C:299:ASP:OD1	1:C:303:ARG:NH2	2.54	0.41
1:F:303:ARG:C	1:F:304:LEU:HD12	2.46	0.41
1:A:135:ASP:OD2	1:A:149:VAL:HG22	2.20	0.41
1:C:25:ALA:O	1:C:28:GLU:HB2	2.21	0.41
1:C:210:PHE:HB3	1:C:242:VAL:CG1	2.51	0.41
1:D:57:LYS:O	1:D:60:ASP:HB2	2.20	0.41
1:E:106:VAL:O	1:E:108:VAL:HG23	2.20	0.41
1:E:210:PHE:HB3	1:E:242:VAL:CG1	2.51	0.41
1:F:373:ILE:HD12	1:F:453:LEU:HD12	2.02	0.41
1:B:41:PRO:HD3	1:B:196:PHE:CZ	2.56	0.41
1:B:99:THR:CG2	1:B:100:ALA:N	2.81	0.41
1:B:124:VAL:HG12	1:B:175:SER:HB3	2.03	0.41
1:C:29:ARG:N	1:C:35:ARG:NH2	2.68	0.41
1:C:99:THR:O	1:C:100:ALA:HB2	2.20	0.41
1:C:300:ALA:O	1:C:303:ARG:HG3	2.21	0.41
1:C:367:ARG:HH21	1:C:368:ASN:HD21	1.69	0.41
1:C:368:ASN:HD22	1:C:368:ASN:HA	1.64	0.41
1:C:433:ASN:N	1:C:433:ASN:HD22	2.17	0.41
1:D:103:ALA:HB1	1:D:173:GLN:CB	2.47	0.41
1:D:351:LYS:NZ	1:D:351:LYS:HB3	2.35	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:A:59:GLU:CD	1:A:59:GLU:H	2.29	0.41
1:E:179:THR:HG22	1:F:181:VAL:CG2	2.47	0.41
1:E:243:ALA:HB2	1:E:270:HIS:HA	2.03	0.41
1:E:335:LEU:C	1:E:352:ASN:HD21	2.29	0.41
1:F:237:LYS:HB2	1:F:363:ASN:HD21	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:O	1:B:60:ASP:HB2	2.21	0.40
1:C:412:ASN:O	1:C:444:LYS:NZ	2.52	0.40
1:D:124:VAL:HG21	1:D:172:LEU:CD2	2.49	0.40
1:D:288:SER:OG	1:D:289:ASN:N	2.54	0.40
1:E:210:PHE:HB2	1:E:223:PHE:CZ	2.56	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:A:266:ILE:CD1	1:B:190:ASN:CG	2.94	0.40
1:B:289:ASN:HB2	1:B:334:ASP:CG	2.46	0.40
1:C:231:ARG:HD3	1:C:249:TYR:OH	2.21	0.40
1:D:414:ASP:O	1:D:416:THR:N	2.54	0.40
1:F:26:ALA:HB2	1:F:400:TYR:CD1	2.56	0.40
1:F:143:VAL:O	1:F:143:VAL:HG13	2.20	0.40
1:F:356:ARG:CG	1:F:356:ARG:NH1	2.84	0.40
1:A:289:ASN:HB2	1:A:334:ASP:CG	2.46	0.40
1:C:424:ASN:C	1:C:426:ASN:N	2.77	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:59:GLU:CD	1:F:59:GLU:H	2.29	0.40
1:F:189:THR:HG23	1:F:192:ASP:OD2	2.20	0.40
1:F:334:ASP:CG	1:F:352:ASN:HB2	2.47	0.40
1:A:18:ILE:CD1	1:A:372:ALA:HA	2.50	0.40
1:B:99:THR:O	1:B:100:ALA:HB2	2.21	0.40
1:B:143:VAL:O	1:B:143:VAL:HG13	2.21	0.40
1:B:251:GLY:O	1:B:252:ILE:HD12	2.21	0.40
1:C:40:LEU:HD23	1:C:41:PRO:HD2	2.02	0.40
1:E:102:LEU:HD23	1:E:103:ALA:H	1.86	0.40
1:E:248:ASP:CG	1:E:340:THR:HG22	2.47	0.40
1:E:414:ASP:O	1:E:416:THR:N	2.54	0.40
1:D:303:ARG:C	1:D:304:LEU:HD12	2.45	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

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	298/460 (65%)	254 (85%)	34 (11%)	10 (3%)	3	18
1	B	433/460 (94%)	370 (86%)	53 (12%)	10 (2%)	5	25
1	C	436/460 (95%)	371 (85%)	51 (12%)	14 (3%)	3	19
1	D	432/460 (94%)	359 (83%)	60 (14%)	13 (3%)	3	20
1	E	429/460 (93%)	370 (86%)	45 (10%)	14 (3%)	3	19
1	F	433/460 (94%)	373 (86%)	48 (11%)	12 (3%)	4	21
All	All	2461/2760 (89%)	2097 (85%)	291 (12%)	73 (3%)	3	20

All (73) 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
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	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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	336 (90%)	36 (10%)	8	28
1	B	368/383 (96%)	329 (89%)	39 (11%)	6	24
1	C	370/383 (97%)	329 (89%)	41 (11%)	6	22
1	D	367/383 (96%)	329 (90%)	38 (10%)	7	25
1	E	364/383 (95%)	323 (89%)	41 (11%)	5	21
1	F	368/383 (96%)	329 (89%)	39 (11%)	6	24
All	All	2209/2298 (96%)	1975 (89%)	234 (11%)	6	24

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	38	VAL
1	A	40	LEU
1	A	56	ASN
1	A	59	GLU
1	A	65	LEU
1	A	75	LEU
1	A	102	LEU
1	A	121	THR
1	A	137	THR
1	A	142	GLU
1	A	172	LEU
1	A	174	GLN

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Mol	Chain	Res	Type
1	A	178	THR
1	A	179	THR
1	A	185	ASP
1	A	186	GLN
1	A	189	THR
1	A	191	LEU
1	A	242	VAL
1	A	245	MSE
1	A	285	MSE
1	A	311	GLU
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
1	A	391	GLN
1	A	447	PHE
1	A	448	THR
1	B	21	ASN
1	B	28	GLU
1	B	35	ARG
1	B	37	THR
1	B	38	VAL
1	B	40	LEU
1	B	56	ASN
1	B	59	GLU
1	B	65	LEU
1	B	75	LEU
1	B	102	LEU
1	B	121	THR
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

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Mol	Chain	Res	Type
1	B	186	GLN
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	311	GLU
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
1	C	18	ILE
1	C	28	GLU
1	C	35	ARG
1	C	38	VAL
1	C	40	LEU
1	C	45	SER
1	C	56	ASN
1	C	59	GLU
1	C	65	LEU
1	C	75	LEU
1	C	102	LEU
1	C	121	THR
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	186	GLN
1	C	189	THR
1	C	191	LEU

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Mol	Chain	Res	Type
1	C	230	MSE
1	C	242	VAL
1	C	245	MSE
1	C	285	MSE
1	C	303	ARG
1	C	311	GLU
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
1	D	38	VAL
1	D	45	SER
1	D	56	ASN
1	D	59	GLU
1	D	65	LEU
1	D	75	LEU
1	D	91	ARG
1	D	102	LEU
1	D	121	THR
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	186	GLN
1	D	189	THR
1	D	191	LEU
1	D	230	MSE
1	D	242	VAL
1	D	245	MSE

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Mol	Chain	Res	Type
1	D	280	ASP
1	D	284	SER
1	D	285	MSE
1	D	311	GLU
1	D	325	ARG
1	D	333	GLN
1	D	336	ASN
1	D	350	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	28	GLU
1	E	34	GLU
1	E	38	VAL
1	E	40	LEU
1	E	56	ASN
1	E	59	GLU
1	E	65	LEU
1	E	75	LEU
1	E	102	LEU
1	E	121	THR
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	186	GLN
1	E	189	THR
1	E	191	LEU
1	E	230	MSE
1	E	242	VAL
1	E	245	MSE
1	E	285	MSE
1	E	325	ARG
1	E	333	GLN

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Mol	Chain	Res	Type
1	E	336	ASN
1	E	345	LYS
1	E	350	ARG
1	E	353	LYS
1	E	354	ILE
1	E	363	ASN
1	E	364	ASP
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	29	ARG
1	F	35	ARG
1	F	37	THR
1	F	38	VAL
1	F	40	LEU
1	F	56	ASN
1	F	59	GLU
1	F	65	LEU
1	F	75	LEU
1	F	102	LEU
1	F	121	THR
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	186	GLN
1	F	189	THR
1	F	191	LEU
1	F	230	MSE
1	F	242	VAL
1	F	245	MSE
1	F	280	ASP
1	F	285	MSE
1	F	290	THR
1	F	311	GLU

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Mol	Chain	Res	Type
1	F	325	ARG
1	F	333	GLN
1	F	336	ASN
1	F	348	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) 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	190	ASN
1	A	254	ASN
1	A	289	ASN
1	A	314	GLN
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	388	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	190	ASN
1	B	254	ASN

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Mol	Chain	Res	Type
1	B	270	HIS
1	B	289	ASN
1	B	314	GLN
1	B	315	ASN
1	B	333	GLN
1	B	336	ASN
1	B	363	ASN
1	B	368	ASN
1	B	380	ASN
1	B	388	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	190	ASN
1	C	254	ASN
1	C	289	ASN
1	C	314	GLN
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	388	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	314	GLN

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Mol	Chain	Res	Type
1	D	315	ASN
1	D	333	GLN
1	D	336	ASN
1	D	363	ASN
1	D	368	ASN
1	D	380	ASN
1	D	388	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	190	ASN
1	E	254	ASN
1	E	289	ASN
1	E	314	GLN
1	E	315	ASN
1	E	333	GLN
1	E	336	ASN
1	E	363	ASN
1	E	380	ASN
1	E	388	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	190	ASN
1	F	254	ASN
1	F	289	ASN
1	F	314	GLN
1	F	315	ASN
1	F	333	GLN
1	F	336	ASN
1	F	363	ASN
1	F	368	ASN
1	F	380	ASN

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Mol	Chain	Res	Type
1	F	388	ASN
1	F	391	GLN
1	F	405	GLN
1	F	424	ASN
1	F	433	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	436/460 (94%)	0.33	27 (6%) 26 18	13, 46, 89, 107	0
1	B	431/460 (93%)	0.16	5 (1%) 76 58	21, 53, 95, 109	0
1	C	434/460 (94%)	0.31	24 (5%) 30 21	15, 50, 92, 109	0
1	D	430/460 (93%)	0.28	14 (3%) 49 33	18, 55, 95, 110	0
1	E	427/460 (92%)	0.27	5 (1%) 76 58	25, 57, 98, 111	0
1	F	431/460 (93%)	0.15	5 (1%) 76 58	17, 52, 92, 109	0
All	All	2589/2760 (93%)	0.25	80 (3%) 51 35	13, 53, 95, 111	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	127	ASN	7.7
1	C	129	VAL	7.7
1	A	129	VAL	6.7
1	A	128	VAL	5.5
1	F	128	VAL	5.0
1	C	128	VAL	4.6
1	F	149	VAL	4.6
1	C	130	ASP	4.4
1	A	149	VAL	4.2
1	A	172	LEU	3.6
1	A	155	GLU	3.5
1	C	150	VAL	3.4
1	C	324	ALA	3.4
1	A	127	ASN	3.4
1	A	135	ASP	3.3
1	C	216	ASP	3.3
1	D	106	VAL	3.3
1	C	153	ALA	3.2
1	A	447	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	130	ASP	3.1
1	E	129	VAL	3.1
1	C	149	VAL	3.1
1	C	154	SER	3.1
1	E	153	ALA	3.0
1	A	151	GLY	3.0
1	A	133	LYS	3.0
1	D	233	GLU	2.9
1	C	134	LYS	2.9
1	B	190	ASN	2.9
1	C	124	VAL	2.9
1	C	135	ASP	2.7
1	D	129	VAL	2.7
1	F	129	VAL	2.7
1	A	157	ILE	2.7
1	A	156	LEU	2.6
1	A	106	VAL	2.6
1	C	151	GLY	2.6
1	B	447	PHE	2.6
1	B	380	ASN	2.5
1	C	168	SER	2.5
1	D	383	ILE	2.5
1	A	374	LYS	2.5
1	D	453	LEU	2.5
1	A	229	ARG	2.5
1	F	447	PHE	2.4
1	C	172	LEU	2.4
1	E	172	LEU	2.4
1	A	417	ALA	2.4
1	D	414	ASP	2.3
1	A	124	VAL	2.3
1	E	128	VAL	2.3
1	C	133	LYS	2.3
1	A	150	VAL	2.3
1	D	102	LEU	2.3
1	C	125	ASP	2.3
1	C	131	SER	2.3
1	D	172	LEU	2.2
1	A	109	THR	2.2
1	C	447	PHE	2.2
1	C	233	GLU	2.2
1	B	128	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	36	GLY	2.2
1	A	125	ASP	2.2
1	D	447	PHE	2.2
1	A	131	SER	2.2
1	A	126	GLU	2.2
1	B	153	ALA	2.1
1	F	127	ASN	2.1
1	D	378	ASP	2.1
1	C	136	VAL	2.1
1	D	393	ILE	2.1
1	C	132	SER	2.1
1	D	150	VAL	2.1
1	A	171	GLU	2.1
1	A	301	THR	2.1
1	C	103	ALA	2.1
1	D	333	GLN	2.1
1	A	284	SER	2.0
1	D	166	THR	2.0
1	E	167	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.