Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 01:13 AM EDT

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 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 (i) 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 (i)) were used in the production of this report:

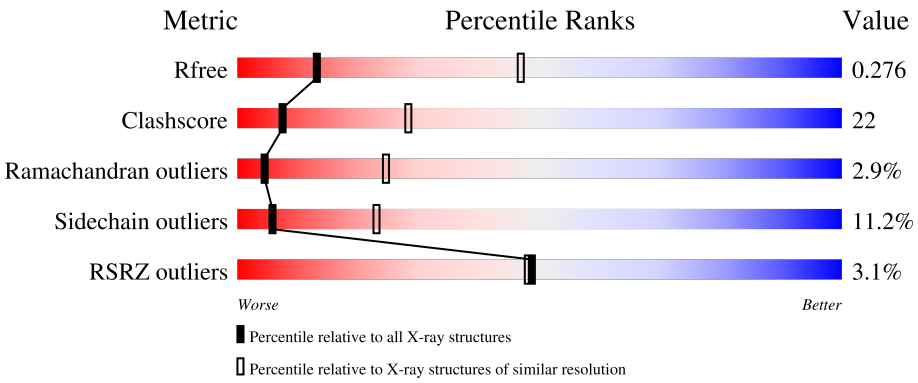
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	%, 55%, 35%, 6%, •
1	B	460	2%, 53%, 35%, 7%, 5%
1	C	460	3%, 53%, 35%, 7%, 5%
1	D	460	4%, 53%, 36%, 6%, 6%

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Validation Pipeline (wwPDB-VP) : 2.37.1

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Mol	Chain	Length	Quality of chain
1	E	460	5% 52% 34% 8% 6%
1	F	460	2% 55% 33% 6% 5%

2 Entry composition (i)

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

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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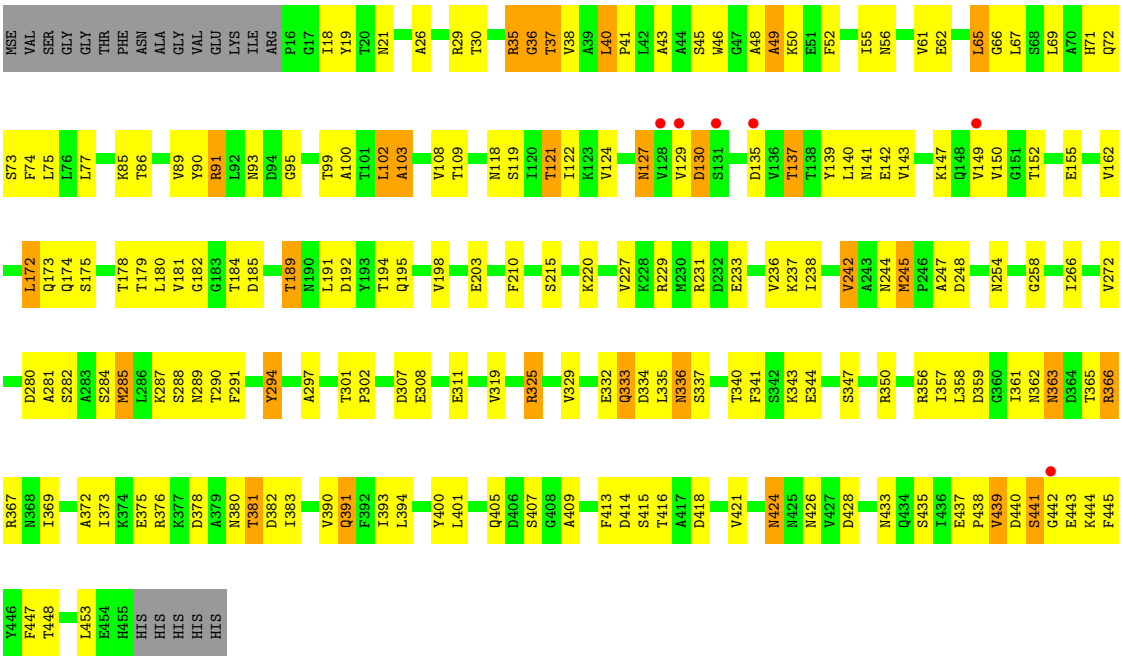
Chain	Residue	Modelled	Actual	Comment	Reference
C	454	GLU	-	EXPRESSION TAG	UNP Q92CB1
C	455	HIS	-	EXPRESSION TAG	UNP Q92CB1
C	456	HIS	-	EXPRESSION TAG	UNP Q92CB1
C	457	HIS	-	EXPRESSION TAG	UNP Q92CB1
C	458	HIS	-	EXPRESSION TAG	UNP Q92CB1
C	459	HIS	-	EXPRESSION TAG	UNP Q92CB1
C	460	HIS	-	EXPRESSION TAG	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 (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.

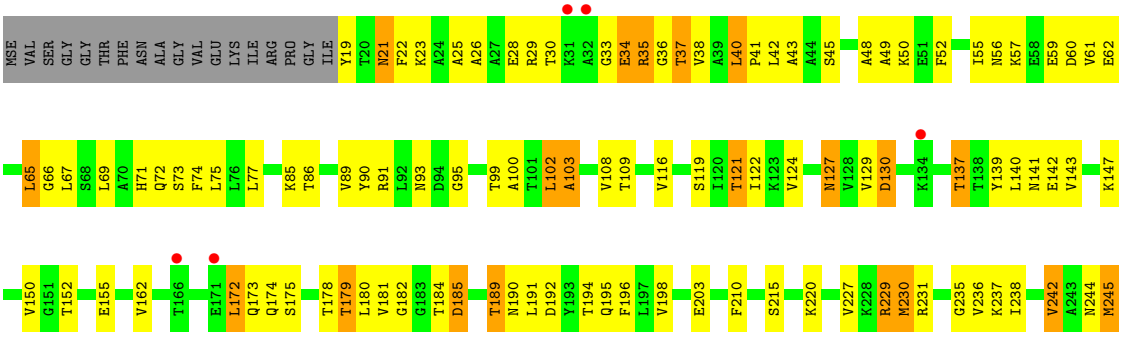
- Molecule 1: Lin1278 protein

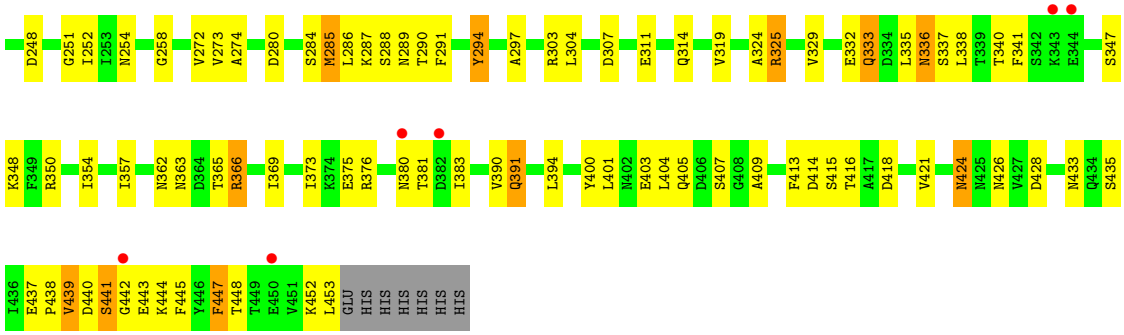
Chain A:



- Molecule 1: Lin1278 protein

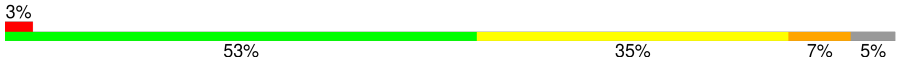
Chain B:

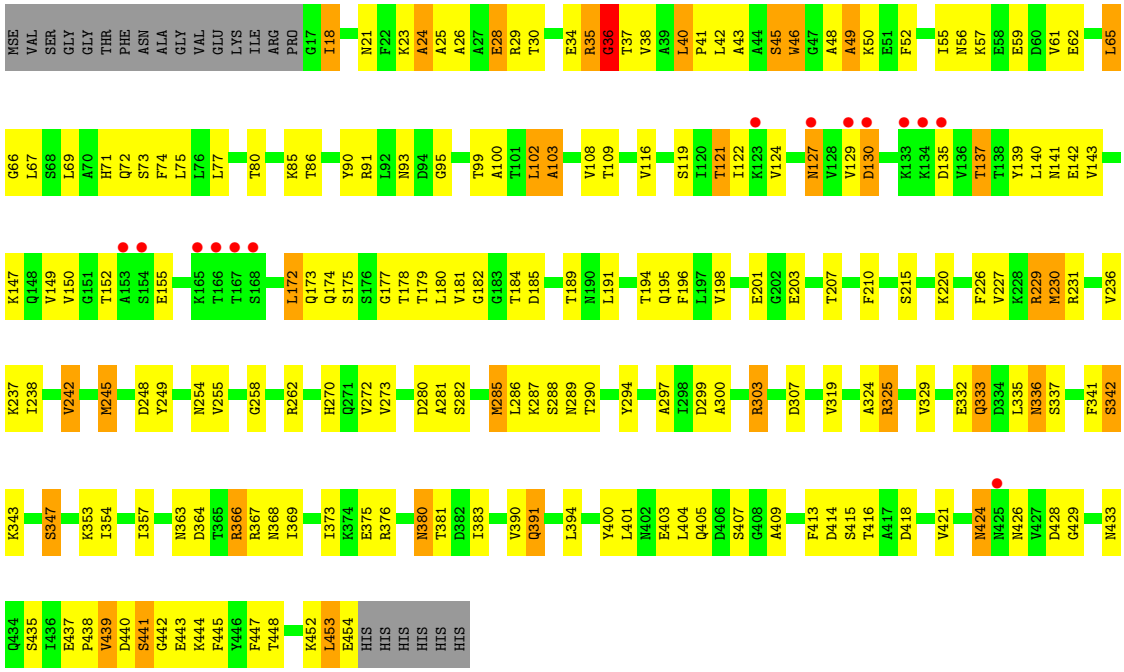




• Molecule 1: Lin1278 protein

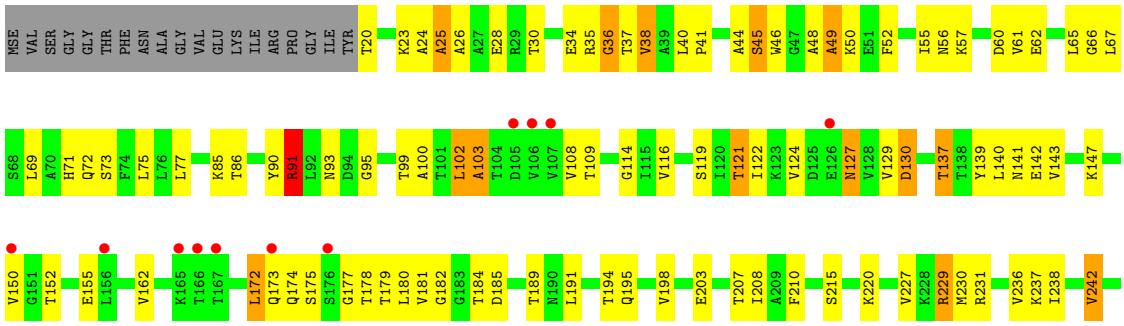
Chain C:

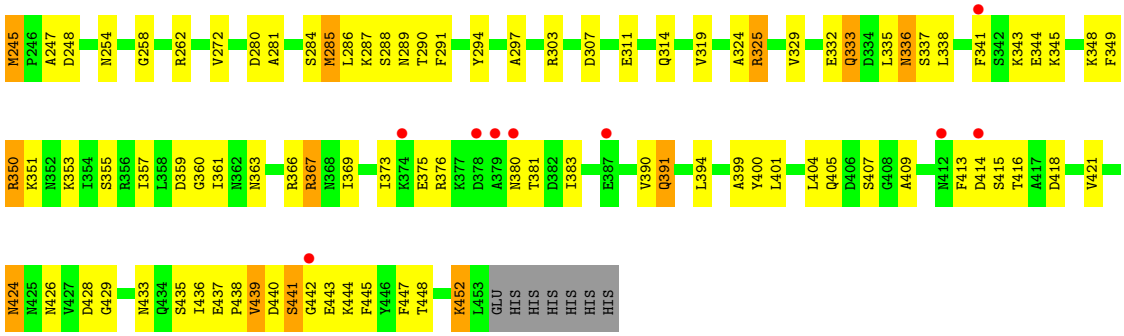




• Molecule 1: Lin1278 protein

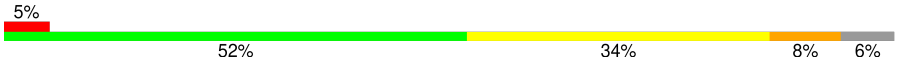
Chain D:

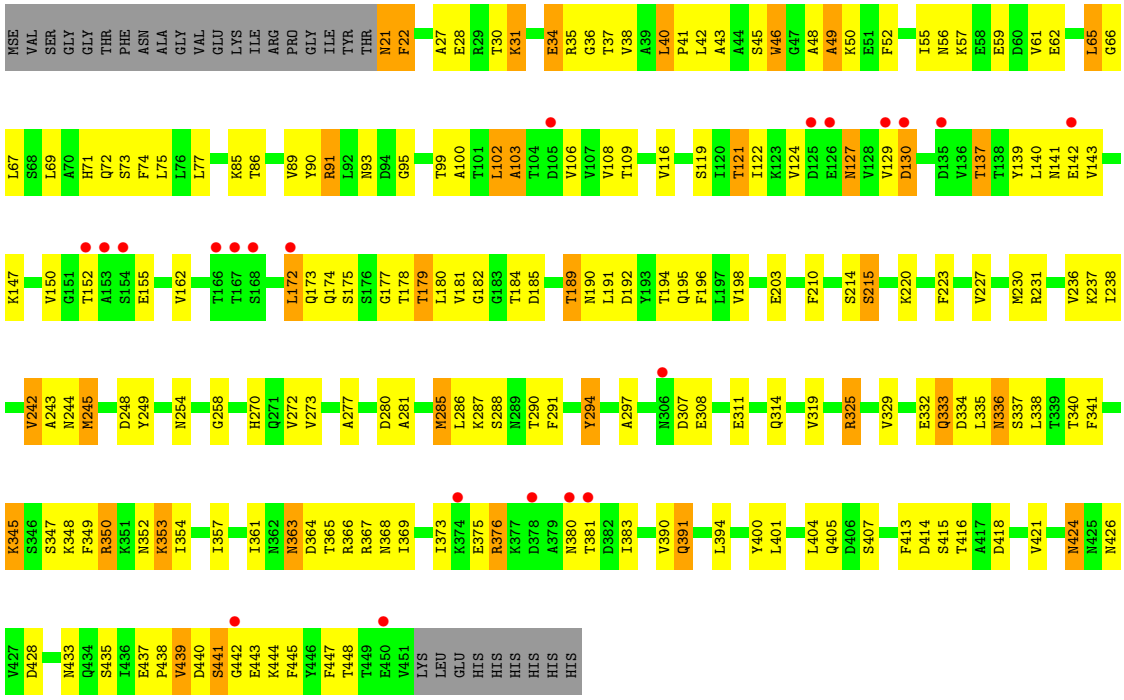




- Molecule 1: Lin1278 protein

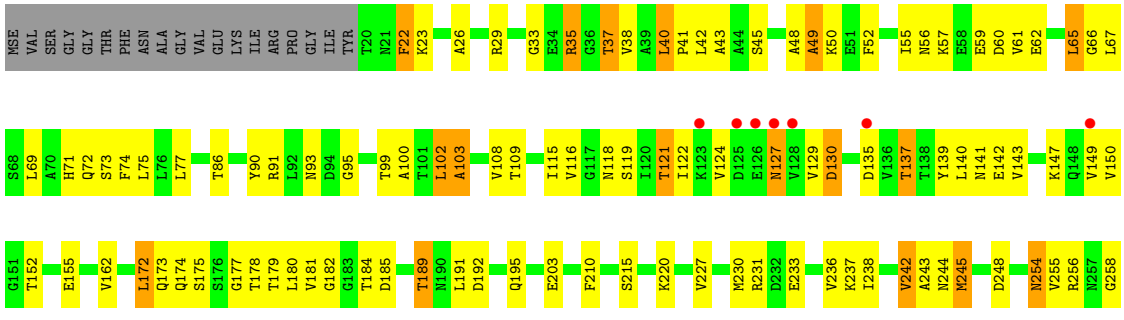
Chain E:

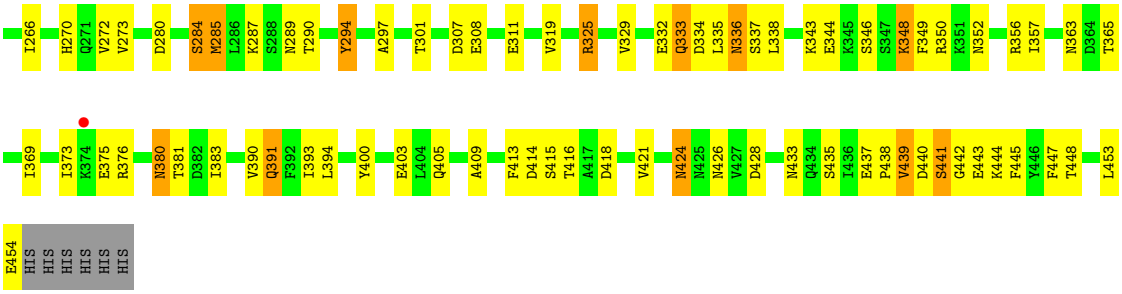




- Molecule 1: Lin1278 protein

Chain F:




I266
H270
Q271
V272
V273
D280
S284
M285
L286
K287
S288
N289
T290
Y294
A297
T301
D307
E308
E311
V319
R325
V329
E332
Q333
D334
L335
N336
S337
L338
K343
E344
K345
S346
S347
K348
F349
R350
K351
N352
R356
I357
N363
D364
T365
I369
I373
K374
E375
R376
N380
T381
D382
I383
V390
Q391
F392
I393
L394
Y400
E403
L404
Q405
A409
F413
D414
S415
T416
A417
D418
V421
N424
N425
N426
V427
D428
N433
Q434
S435
I436
E437
P438
V439
D440
S441
G442
E443
K444
F445
Y446
F447
T448
L453
E454
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.28 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 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	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

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 22.

All (889) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:GLN:NE2	1:A:413:PHE:H	1.98	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
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: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: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: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: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: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:A:48:ALA:O	1:A:49:ALA:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:B:424:ASN:C	1:B:426:ASN:H	2.08	0.57
1:A:340:THR:HG23	1:A:340:THR:O	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: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:343:LYS:HZ1	1:A:344:GLU:HG3	1.71	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:23:LYS:C	1:C:25:ALA:H	2.09	0.55
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
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:C:424:ASN:C	1:C:426:ASN:H	2.09	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:VAL:O	1:C:130:ASP:HB2	2.12	0.50
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: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: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: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: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: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: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: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: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:A:336:ASN:C	1:A:336:ASN:HD22	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:VAL:HG13	1:D:421:VAL:HB	1.94	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:E:345:LYS:HD2	1:E:345:LYS:C	2.32	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:B:124:VAL:HG13	1:B:175:SER:N	2.28	0.48
1:D:124:VAL:HG13	1:D:175:SER:N	2.28	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:C:66:GLY:C	1:C:67:LEU:HD22	2.33	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: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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:23:LYS:HZ2	1:B:403:GLU:HG2	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: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
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: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: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: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: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:E:55:ILE:O	1:E:55:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:50:LYS:HZ1	1:B:195:GLN:HG3	1.79	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: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: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: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: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: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: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:71:HIS:CE1	1:C:73:SER:HG	2.34	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLY:C	1:B:67:LEU:HD22	2.37	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: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:C:237:LYS:H	1:C:363:ASN:HD21	1.64	0.45
1:E:66:GLY:C	1:E:67:LEU:HD22	2.36	0.45
1:E:102:LEU:HD12	1:E:108:VAL:HG21	1.97	0.45
1:D:297:ALA:HB3	1:D:329:VAL:CG1	2.46	0.45
1:F:71:HIS:ND1	1:F:72:GLN:N	2.64	0.45
1:F:336:ASN:C	1:F:336:ASN:HD22	2.19	0.45
1:E:336:ASN:C	1:E:336:ASN:HD22	2.19	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: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: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:288:SER:HB2	1:C:353:LYS:HD2	1.97	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:45:SER:O	1:A:46:TRP:HB2	2.17	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:B:248:ASP:CG	1:B:340:THR:HG22	2.36	0.45
1:D:44:ALA:HB3	1:D:91:ARG:CG	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:71:HIS:ND1	1:B:72:GLN:N	2.65	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: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: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:C:18:ILE:HD12	1:C:18:ILE:N	2.30	0.44
1:C:336:ASN:C	1:C:336:ASN:HD22	2.20	0.44
1:E:347:SER:C	1:E:349:PHE:H	2.20	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: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:303:ARG:C	1:B:304:LEU:HD12	2.38	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: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:D:336:ASN:C	1:D:336:ASN:HD22	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:71:HIS:CE1	1:D:73:SER:HG	2.35	0.44
1:F:343:LYS:HG3	1:F:344:GLU:N	2.33	0.44
1:A:414:ASP:C	1:A:416:THR:N	2.71	0.44
1:B:336:ASN:C	1:B:336:ASN:HD22	2.22	0.44
1:B:414:ASP:C	1:B:416:THR:N	2.71	0.44
1:D:360:GLY:O	1:D:361:ILE:C	2.55	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:A:66:GLY:C	1:A:67:LEU:HD22	2.39	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:C:194:THR:O	1:C:198:VAL:HG23	2.18	0.44
1:E:71:HIS:ND1	1:E:72:GLN:N	2.66	0.44
1:F:127:ASN:HB3	1:F:130:ASP:O	2.18	0.44
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:F:50:LYS:HZ3	1:F:195:GLN:HG3	1.82	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: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: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: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:A:43:ALA:HB1	1:A:93:ASN:HD22	1.82	0.43
1:B:100:ALA:HB2	1:B:180:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:66:GLY:C	1:D:67:LEU:HD22	2.39	0.43
1:D:290:THR:O	1:D:291:PHE:CB	2.66	0.43
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:229:ARG:HD2	1:C:201:GLU:OE1	2.19	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:181:VAL:HG22	1:B:182:GLY:N	2.34	0.43
1:C:414:ASP:C	1:C:416:THR:N	2.72	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:B:220:LYS:HD3	1:B:245:MSE:HG2	2.01	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: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: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: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:D:30:THR:HG23	1:D:286:LEU:CD1	2.49	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:F:66:GLY:C	1:F:67:LEU:HD22	2.40	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: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: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
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:D:335:LEU:HD22	1:D:350:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:GLN:CD	1:E:335:LEU:HD21	2.38	0.42
1:B:33:GLY:O	1:B:34:GLU:C	2.58	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: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: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:C:438:PRO:O	1:C:439:VAL:C	2.58	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:E:414:ASP:C	1:E:416:THR:N	2.73	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:A:358:LEU:O	1:A:359:ASP:C	2.56	0.42
1:B:103:ALA:HB1	1:B:173:GLN:CB	2.46	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:PHE:HB3	1:D:242:VAL:CG1	2.49	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: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: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: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:F:438:PRO:O	1:F:439:VAL:C	2.58	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:A:381:THR:O	1:A:382:ASP:C	2.59	0.41
1:B:119:SER:HB3	1:B:141:ASN:HD21	1.85	0.41
1:B:235:GLY:C	1:B:366:ARG:HH12	2.22	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:E:194:THR:O	1:E:198:VAL:HG23	2.20	0.41
1:F:414:ASP:C	1:F:416:THR:N	2.71	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:A:333:GLN:CD	1:A:335:LEU:HD21	2.41	0.41
1:D:20:THR:C	1:D:24:ALA:HB2	2.41	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: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:E:36:GLY:HA3	1:E:281:ALA:O	2.20	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

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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:F:256:ARG:HB3	1:F:319:VAL:HG12	2.01	0.41
1:F:414:ASP:C	1:F:416:THR:H	2.24	0.41
1:B:26:ALA:HB1	1:B:403:GLU:HB3	2.02	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:229:ARG:O	1:B:230:MSE:C	2.59	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:A:135:ASP:OD2	1:A:149:VAL:HG22	2.20	0.41
1:A:189:THR:HG23	1:A:192:ASP:CG	2.41	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:E:438:PRO:O	1:E:439:VAL:C	2.58	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:D:414:ASP:C	1:D:416:THR:N	2.74	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:F:237:LYS:HB2	1:F:363:ASN:HD21	1.82	0.41
1:B:57:LYS:O	1:B:60:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ASP:C	1:C:416:THR:H	2.24	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: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: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: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: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:A:18:ILE:CD1	1:A:372:ALA:HA	2.50	0.40
1:A:247:ALA:O	1:A:248:ASP:C	2.59	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:D:247:ALA:O	1:D:248:ASP:C	2.60	0.40
1:E:102:LEU:HD23	1:E:103:ALA:H	1.86	0.40
1:E:414:ASP:O	1:E:416:THR:N	2.54	0.40
1:B:189:THR:HG23	1:B:192:ASP:CG	2.42	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	438/460 (95%)	372 (85%)	54 (12%)	12 (3%)	5 26
1	B	433/460 (94%)	370 (86%)	53 (12%)	10 (2%)	6 29
1	C	436/460 (95%)	371 (85%)	51 (12%)	14 (3%)	4 22
1	D	432/460 (94%)	359 (83%)	60 (14%)	13 (3%)	4 24
1	E	429/460 (93%)	370 (86%)	45 (10%)	14 (3%)	4 22
1	F	433/460 (94%)	373 (86%)	48 (11%)	12 (3%)	5 25
All	All	2601/2760 (94%)	2215 (85%)	311 (12%)	75 (3%)	4 24

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
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

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Mol	Chain	Res	Type
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
1	B	244	ASN
1	D	177	GLY

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Mol	Chain	Res	Type
1	C	177	GLY
1	F	177	GLY
1	E	177	GLY

5.3.2 Protein sidechains (i)

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%)	6	24
1	B	368/383 (96%)	329 (89%)	39 (11%)	6	25
1	C	370/383 (97%)	329 (89%)	41 (11%)	6	23
1	D	367/383 (96%)	327 (89%)	40 (11%)	6	24
1	E	364/383 (95%)	320 (88%)	44 (12%)	5	20
1	F	368/383 (96%)	325 (88%)	43 (12%)	5	21
All	All	2209/2298 (96%)	1962 (89%)	247 (11%)	6	23

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Sometimes 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	436/460 (94%)	-0.02	6 (1%)	75	75	13, 46, 89, 107	0
1	B	431/460 (93%)	0.04	11 (2%)	56	53	21, 53, 95, 109	0
1	C	434/460 (94%)	0.05	14 (3%)	47	46	15, 50, 92, 109	0
1	D	430/460 (93%)	0.23	20 (4%)	31	29	18, 55, 95, 110	0
1	E	427/460 (92%)	0.23	21 (4%)	29	27	25, 57, 98, 111	0
1	F	431/460 (93%)	-0.02	8 (1%)	66	65	17, 52, 92, 109	0
All	All	2589/2760 (93%)	0.08	80 (3%)	49	48	13, 53, 95, 111	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	106	VAL	5.6
1	C	127	ASN	5.4
1	E	153	ALA	5.0
1	D	107	VAL	4.8
1	B	380	ASN	4.7
1	F	128	VAL	4.3
1	C	154	SER	4.3
1	D	378	ASP	4.1
1	C	129	VAL	4.0
1	E	380	ASN	3.8
1	C	130	ASP	3.8
1	D	380	ASN	3.7
1	E	167	THR	3.7
1	F	149	VAL	3.6
1	D	442	GLY	3.6
1	E	378	ASP	3.5
1	C	167	THR	3.4
1	D	166	THR	3.3
1	A	128	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	125	ASP	3.1
1	A	131	SER	3.1
1	E	130	ASP	3.0
1	E	306	ASN	3.0
1	D	167	THR	3.0
1	C	134	LYS	2.9
1	F	126	GLU	2.9
1	D	379	ALA	2.8
1	D	176	SER	2.8
1	E	125	ASP	2.8
1	A	135	ASP	2.6
1	E	168	SER	2.6
1	D	374	LYS	2.6
1	D	412	ASN	2.6
1	D	105	ASP	2.5
1	C	165	LYS	2.5
1	B	382	ASP	2.5
1	C	135	ASP	2.5
1	E	166	THR	2.5
1	B	344	GLU	2.5
1	E	381	THR	2.5
1	E	135	ASP	2.5
1	A	129	VAL	2.5
1	E	450	GLU	2.5
1	F	127	ASN	2.5
1	C	168	SER	2.4
1	D	173	GLN	2.4
1	D	165	LYS	2.4
1	B	343	LYS	2.3
1	E	105	ASP	2.3
1	D	126	GLU	2.3
1	C	153	ALA	2.3
1	E	129	VAL	2.3
1	D	387	GLU	2.3
1	B	442	GLY	2.3
1	E	172	LEU	2.3
1	B	450	GLU	2.3
1	E	142	GLU	2.3
1	E	126	GLU	2.2
1	C	123	LYS	2.2
1	C	133	LYS	2.2
1	A	149	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	442	GLY	2.2
1	B	32	ALA	2.2
1	A	442	GLY	2.2
1	F	123	LYS	2.2
1	D	341	PHE	2.2
1	D	414	ASP	2.2
1	B	31	LYS	2.1
1	C	166	THR	2.1
1	E	154	SER	2.1
1	D	150	VAL	2.1
1	E	152	THR	2.1
1	D	156	LEU	2.1
1	B	166	THR	2.1
1	C	425	ASN	2.0
1	F	135	ASP	2.0
1	B	171	GLU	2.0
1	F	374	LYS	2.0
1	B	134	LYS	2.0
1	E	374	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.