



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:35 pm BST

PDB ID : 6ABH
Title : Structure of a natural red emitting luciferase from Phrixothrix hirtus (P1 crystal form)
Authors : Carrasco-Lopez, C.; Panjekar, S.; Naumov, P.; Rabeh, W.
Deposited on : 2018-07-21
Resolution : 3.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

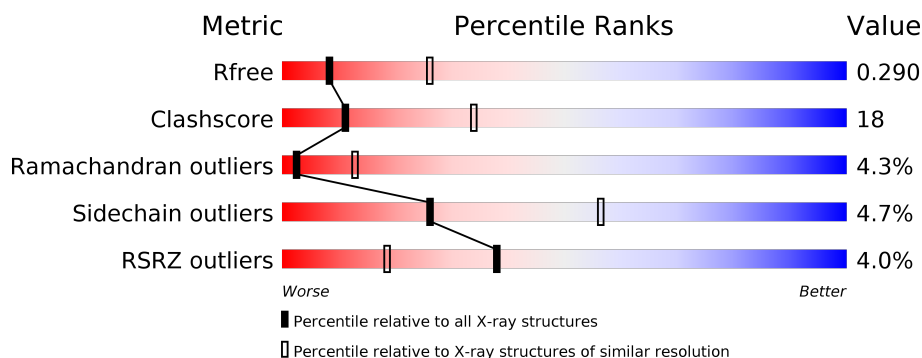
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	546	<div> <div>44%</div> <div>23%</div> <div>•</div> <div>31%</div> </div>
1	B	546	<div>4%</div> <div>48%</div> <div>23%</div> <div>•</div> <div>26%</div>

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Mol	Chain	Length	Quality of chain
1	G	546	<div><div><div>3%</div><div>47%</div><div>24%</div><div>•</div><div>27%</div></div></div>
1	H	546	<div><div><div>3%</div><div>43%</div><div>27%</div><div>•</div><div>27%</div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25451 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.

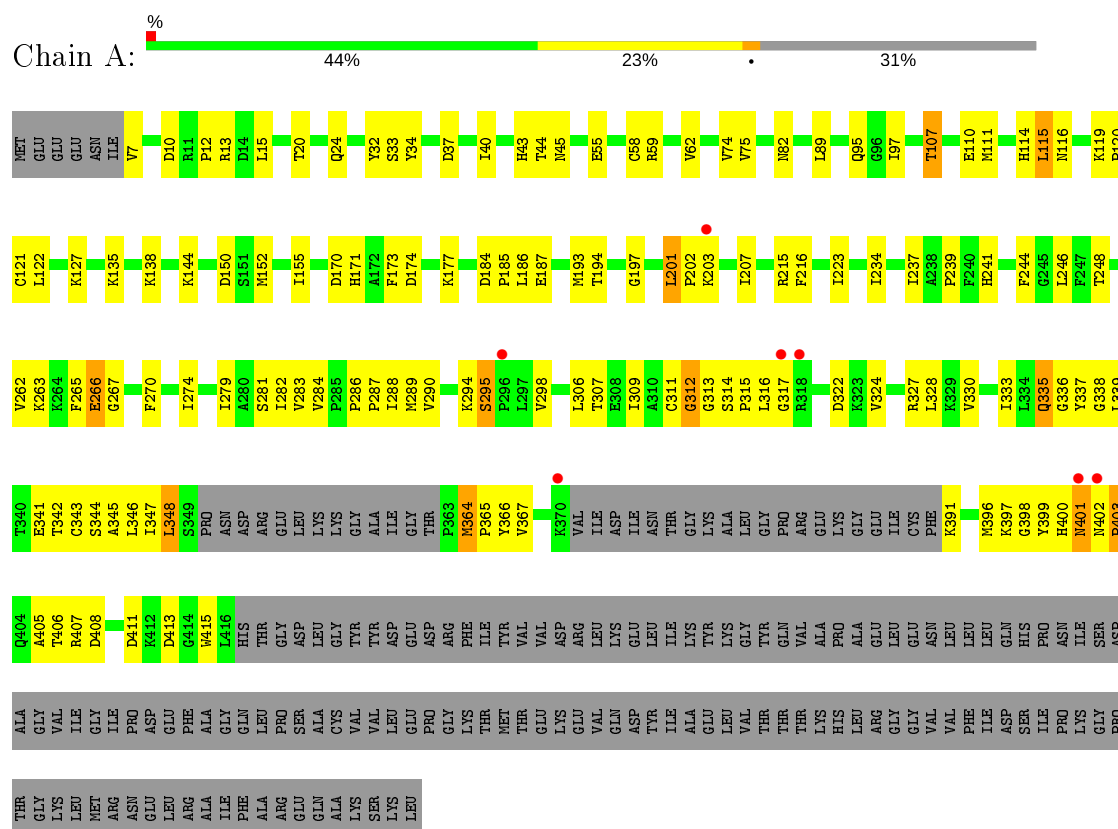
- Molecule 1 is a protein called Red-bioluminescence eliciting luciferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2955	1915	487	535	18			
1	B	405	Total	C	N	O	S	0	0	0
			3170	2047	527	577	19			
1	C	409	Total	C	N	O	S	0	0	0
			3199	2069	531	580	19			
1	D	442	Total	C	N	O	S	0	0	0
			3480	2251	576	634	19			
1	E	398	Total	C	N	O	S	0	0	0
			3110	2011	515	565	19			
1	F	417	Total	C	N	O	S	0	0	0
			3262	2107	541	595	19			
1	G	401	Total	C	N	O	S	0	0	0
			3137	2030	519	570	18			
1	H	400	Total	C	N	O	S	0	0	0
			3138	2028	517	575	18			

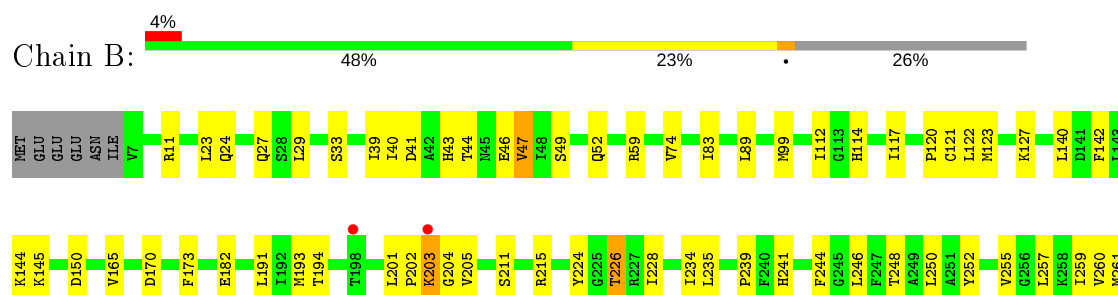
3 Residue-property plots [i](#)

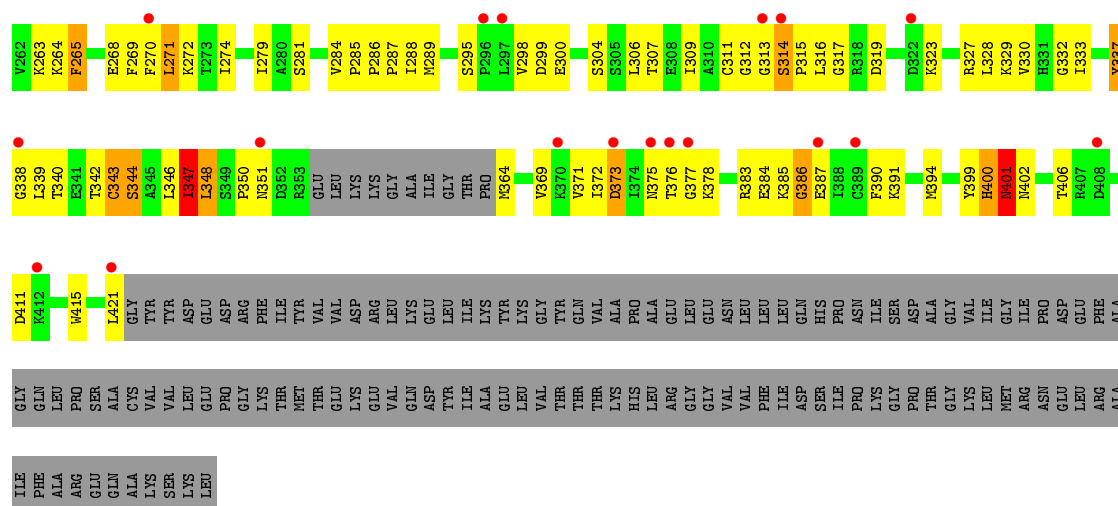
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Red-bioluminescence eliciting luciferase

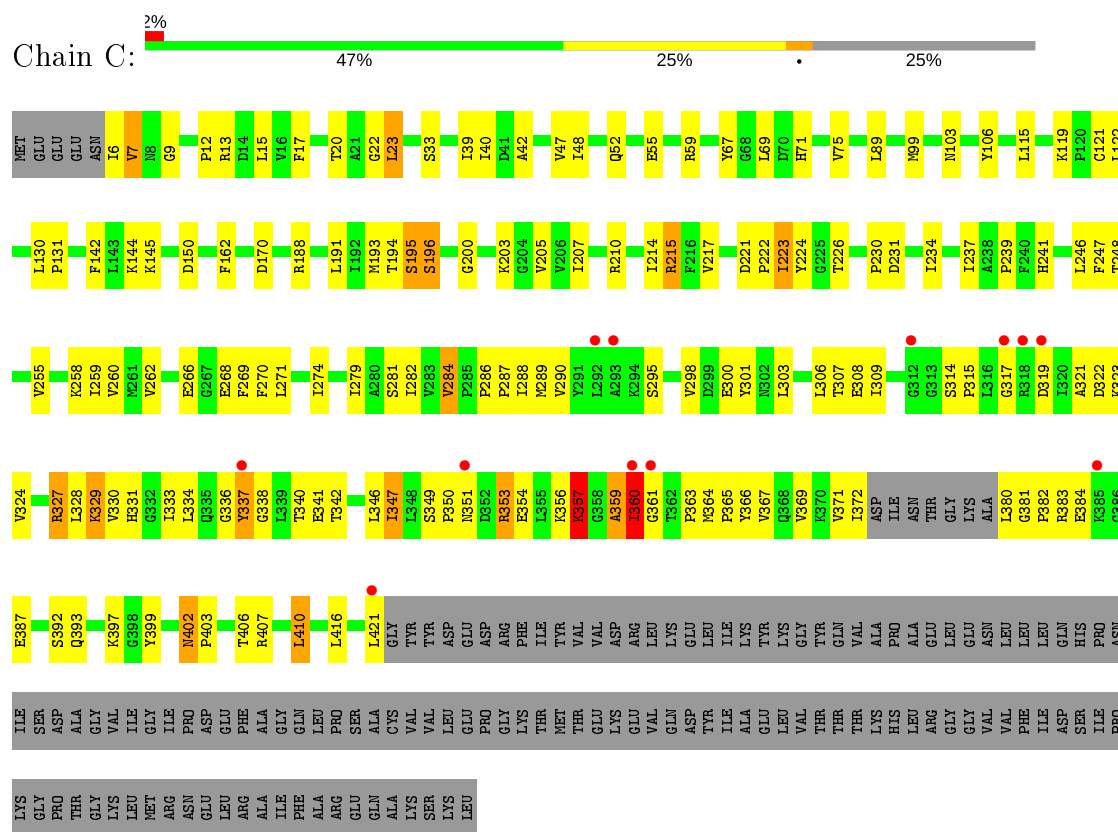


- Molecule 1: Red-bioluminescence eliciting luciferase

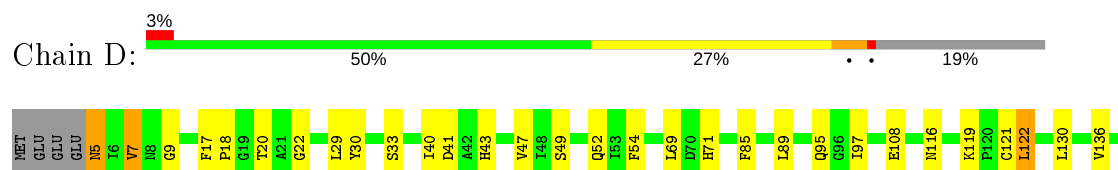


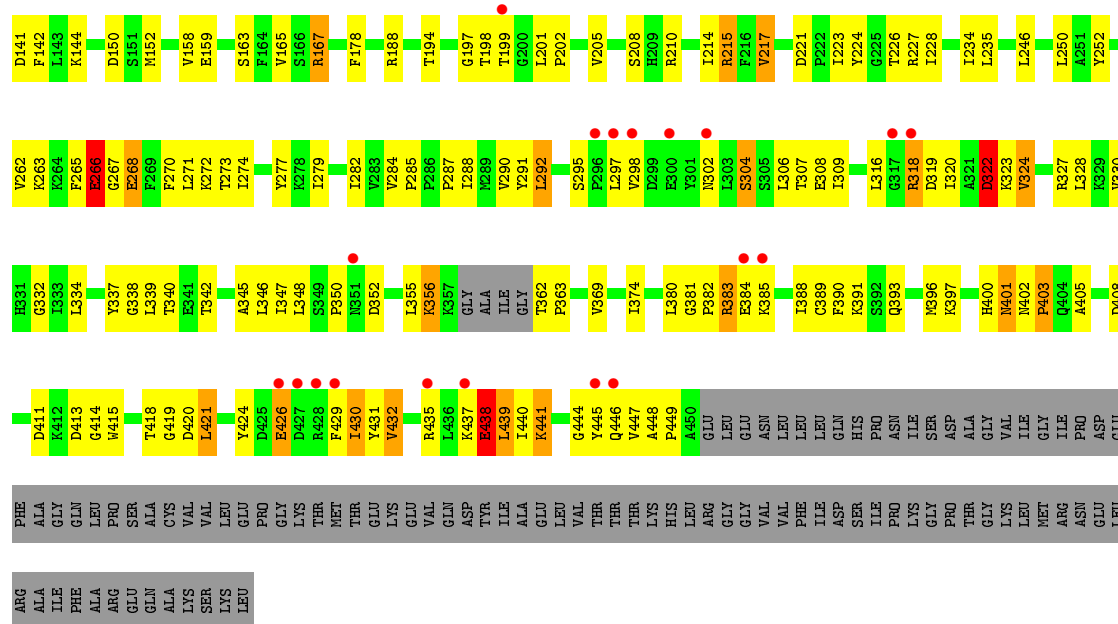


• Molecule 1: Red-bioluminescence eliciting luciferase

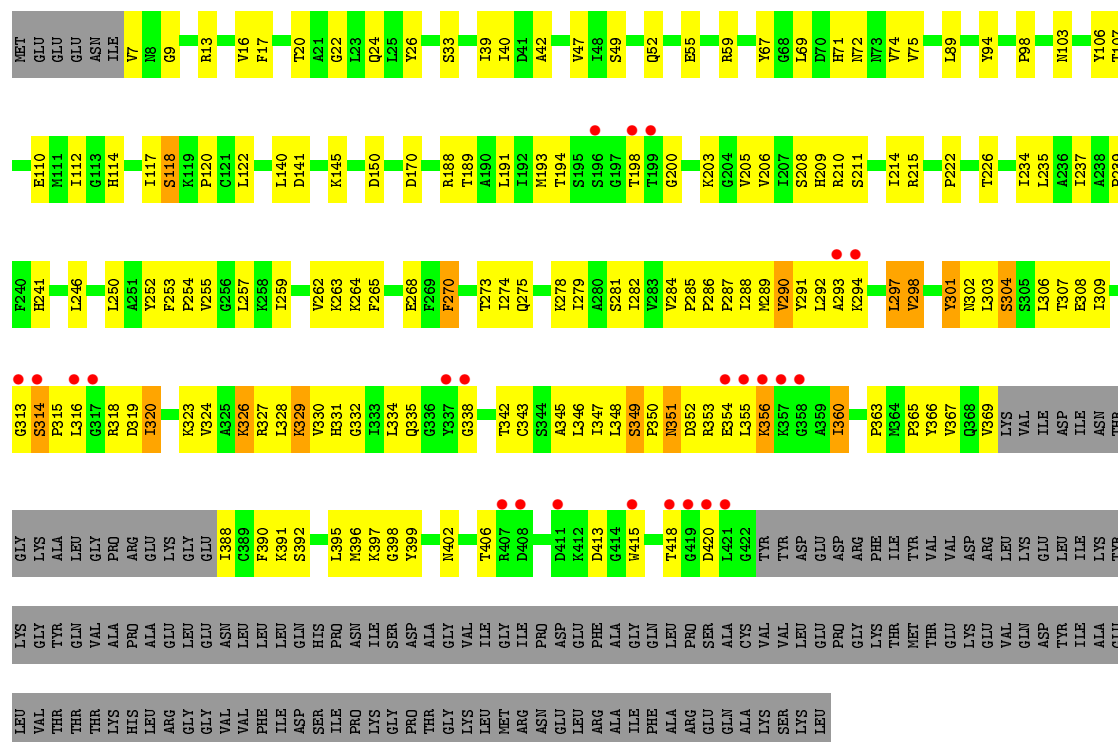
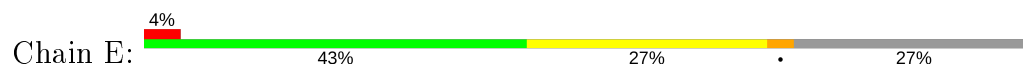


• Molecule 1: Red-bioluminescence eliciting luciferase



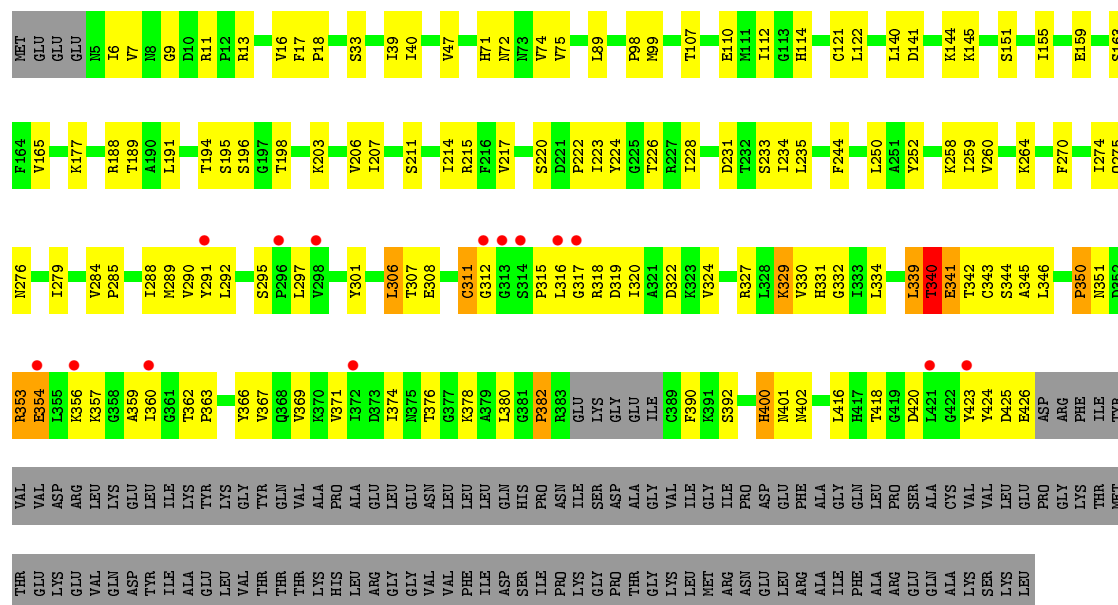


• Molecule 1: Red-bioluminescence eliciting luciferase

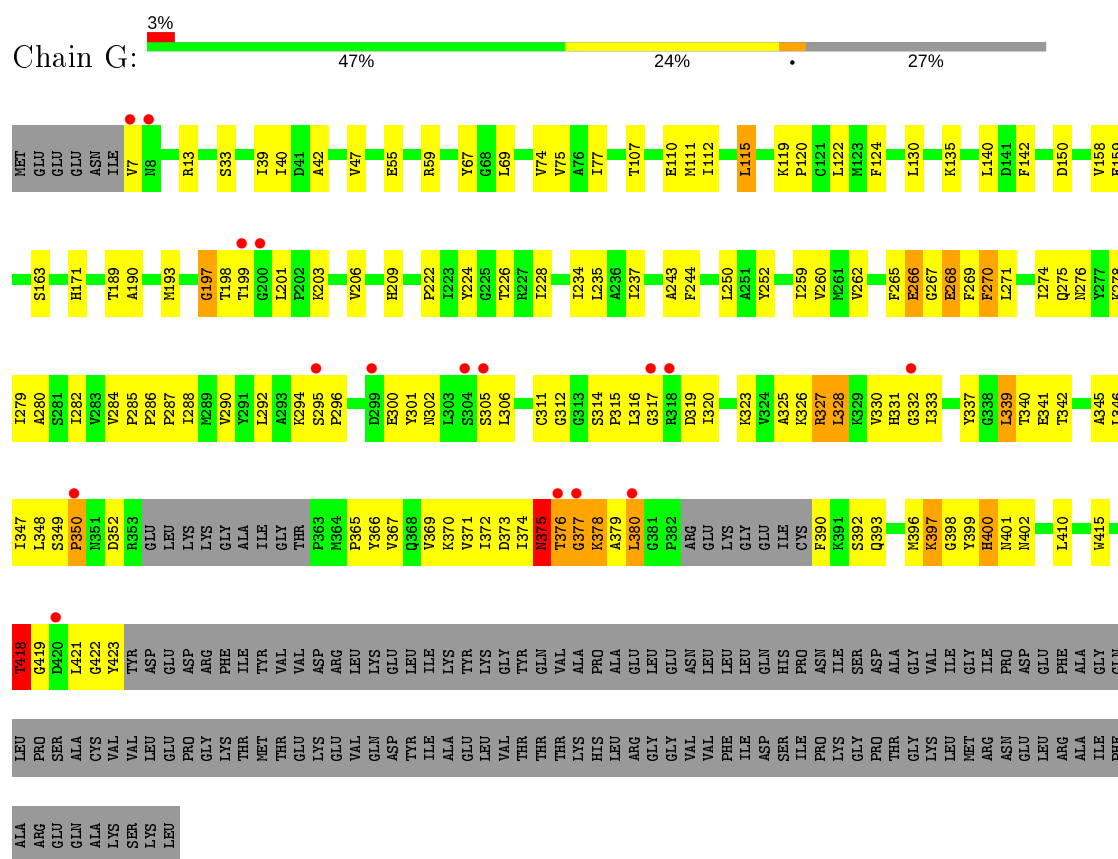


• Molecule 1: Red-bioluminescence eliciting luciferase

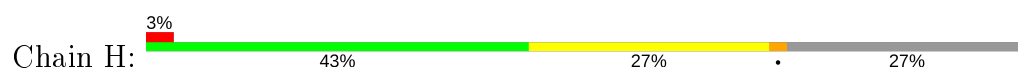




• Molecule 1: Red-bioluminescence eliciting luciferase



• Molecule 1: Red-bioluminescence eliciting luciferase



THR	LEU	MET
ILE	ILE	GLU
ALA	TYR	GLU
GLU	LYS	GLU
LEU	VAL	ASN
GLY	THR	ILE
TYR	THR	V7
GLN	THR	I8
VAL	THR	G9
ALA	LYS	P12
PRO	PRO	R13
ALA	ALA	D14
GLU	ARG	L15
ILE	ARG	V16
CYS	GLY	F17
F390	GLY	F17
Q393	VAL	T20
M394	LEU	A21
I395	LEU	G22
M396	GLN	L25
K397	SER	S33
G398	ILE	D87
Y399	PRO	I40
H400	ASN	D41
M401	LYS	A42
M402	SER	V47
P403	ASP	I48
Q404	ALA	Q52
A405	GLY	E55
T406	VAL	R59
T406	ILE	V74
R407	ILE	F85
D408	GLY	F86
A409	PRO	I89
L410	ASP	I90
L410	GLU	Q95
D413	LEU	G96
G414	PHE	I97
M415	ILE	N103
L416	GLN	Y106
H417	LEU	T107
D420	PRO	E108
L421	SER	R109
G422	ALA	E110
Y423	VAL	M111
Y424	LYS	I112
D425	SER	L115
E426	LYS	K119
D427	LEU	P120
ARG	PRO	L140
PHE	GLY	D141
ILE	LYS	F142
THR	THR	L143
MET	MET	K144
TYR	THR	K145
THR	THR	V146
GLU	THR	I147
ASP	THR	V148
ASP	THR	I149
ASP	THR	D150
ASP	THR	I155
ASP	THR	V161
ASP	THR	F162
ASP	THR	V165
ASP	THR	D170
ASP	THR	H171
ASP	THR	A172
ASP	THR	F173
ASP	THR	D184
ASP	THR	P185
ASP	THR	L186
ASP	THR	E187
ASP	THR	L191
ASP	THR	I192
ASP	THR	M193
ASP	THR	S196
ASP	THR	G197
ASP	THR	T198
ASP	THR	T199
ASP	THR	G200
ASP	THR	L201
ASP	THR	P202
ASP	THR	K203
ASP	THR	G204
ASP	THR	R210
ASP	THR	S211
ASP	THR	T212
ASP	THR	T213
ASP	THR	I214
ASP	THR	R215
ASP	THR	F216
ASP	THR	V217
ASP	THR	P222
ASP	THR	I228
ASP	THR	T232
ASP	THR	S233
ASP	THR	I234
ASP	THR	L235
ASP	THR	A236
ASP	THR	L246
ASP	THR	F247
ASP	THR	L248
ASP	THR	T249
ASP	THR	K249
ASP	THR	L250
ASP	THR	A251
ASP	THR	Y252
ASP	THR	K258
ASP	THR	I259
ASP	THR	V260
ASP	THR	F261
ASP	THR	V262
ASP	THR	F265
ASP	THR	E266
ASP	THR	G267
ASP	THR	E268
ASP	THR	F269
ASP	THR	F270
ASP	THR	L271
ASP	THR	I274
ASP	THR	L279
ASP	THR	A280
ASP	THR	S281
ASP	THR	I282
ASP	THR	V283
ASP	THR	V284
ASP	THR	P285
ASP	THR	P286
ASP	THR	P287
ASP	THR	I288
ASP	THR	M289
ASP	THR	V290
ASP	THR	Y291
ASP	THR	L292
ASP	THR	A293
ASP	THR	K294
ASP	THR	V298
ASP	THR	L303
ASP	THR	S304
ASP	THR	L305
ASP	THR	L306
ASP	THR	I309
ASP	THR	A310
ASP	THR	C311
ASP	THR	V367
ASP	THR	Q368
ASP	THR	VAL
ASP	THR	LYS
ASP	THR	VAL
ASP	THR	ASP
ASP	THR	ARG
ASP	THR	LEU
ASP	THR	LYS
ASP	THR	ILE
ASP	THR	ASP
ASP	THR	ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	105.70Å 121.17Å 129.44Å 61.86° 68.35° 74.17°	Depositor
Resolution (Å)	48.76 – 3.05 48.76 – 3.05	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.76-3.05) 94.2 (48.76-3.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.240 , 0.285 0.258 , 0.290	Depositor DCC
R_{free} test set	955 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å ²)	73.0	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25451	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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	0.59	0/3026	0.77	0/4100
1	B	0.54	0/3245	0.72	0/4398
1	C	0.57	0/3275	0.75	0/4438
1	D	0.62	0/3563	0.78	0/4829
1	E	0.53	0/3185	0.74	0/4318
1	F	0.58	0/3340	0.81	2/4528 (0.0%)
1	G	0.55	0/3213	0.75	0/4356
1	H	0.60	0/3215	0.79	1/4359 (0.0%)
All	All	0.57	0/26062	0.76	3/35326 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	3
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	341	GLU	N-CA-C	-12.20	78.05	111.00
1	H	398	GLY	N-CA-C	-5.69	98.88	113.10
1	F	341	GLU	N-CA-CB	5.18	119.92	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	11	ARG	Sidechain
1	D	167	ARG	Sidechain
1	D	215	ARG	Sidechain
1	D	318	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2955	0	2990	107	0
1	B	3170	0	3205	96	0
1	C	3199	0	3246	116	0
1	D	3480	0	3513	141	0
1	E	3110	0	3143	126	0
1	F	3262	0	3293	102	0
1	G	3137	0	3167	103	0
1	H	3138	0	3150	137	0
All	All	25451	0	25707	915	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 18.

All (915) 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:A:201:LEU:HD22	1:A:202:PRO:CD	1.45	1.47
1:A:201:LEU:CD2	1:A:202:PRO:HD3	1.59	1.30
1:F:340:THR:OG1	1:F:344:SER:HA	1.29	1.29
1:G:370:LYS:HD2	1:G:415:TRP:CE3	1.72	1.24
1:D:319:ASP:O	1:D:323:LYS:HG3	1.43	1.17
1:G:371:VAL:HG11	1:G:380:LEU:CB	1.84	1.06
1:H:311:CYS:H	1:H:335:GLN:HG2	0.97	1.05
1:G:371:VAL:HG11	1:G:380:LEU:CG	1.86	1.05
1:H:311:CYS:N	1:H:335:GLN:HG2	1.72	1.04
1:E:334:LEU:HA	1:E:350:PRO:HG2	1.36	1.01
1:A:201:LEU:HD13	1:A:202:PRO:HD2	1.40	1.01
1:D:295:SER:OG	1:D:297:LEU:HG	1.59	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:TYR:OH	1:D:297:LEU:HD21	1.62	0.99
1:H:337:TYR:CE2	1:H:339:LEU:HG	1.96	0.98
1:A:396:MET:HG2	1:A:398:GLY:H	1.29	0.97
1:A:201:LEU:CD2	1:A:202:PRO:CD	2.29	0.95
1:B:40:ILE:HG12	1:B:47:VAL:HG23	1.46	0.95
1:E:399:TYR:H	1:E:406:THR:HG22	1.29	0.94
1:G:337:TYR:OH	1:G:418:THR:HG22	1.67	0.94
1:C:399:TYR:H	1:C:406:THR:HG22	1.33	0.94
1:F:339:LEU:HD22	1:F:416:LEU:HD21	1.50	0.93
1:A:201:LEU:CD1	1:A:202:PRO:HD2	1.99	0.93
1:G:370:LYS:HD2	1:G:415:TRP:CD2	2.03	0.92
1:G:369:VAL:HG22	1:G:390:PHE:CE1	2.05	0.92
1:E:237:ILE:HD13	1:E:262:VAL:HG23	1.52	0.91
1:C:317:GLY:HA2	1:C:321:ALA:HB2	1.52	0.91
1:B:347:ILE:H	1:B:364:MET:HB2	1.35	0.90
1:F:425:ASP:O	1:F:426:GLU:HG2	1.72	0.90
1:F:425:ASP:O	1:F:426:GLU:CG	2.20	0.89
1:G:370:LYS:CD	1:G:415:TRP:CE3	2.56	0.89
1:F:235:LEU:HB2	1:F:279:ILE:HD13	1.53	0.88
1:E:275:GLN:HG2	1:E:301:TYR:HD1	1.40	0.87
1:H:337:TYR:CD2	1:H:339:LEU:HG	2.09	0.87
1:C:215:ARG:NH1	1:C:248:THR:HG22	1.91	0.85
1:F:400:HIS:O	1:F:402:ASN:N	2.09	0.85
1:E:292:LEU:HD13	1:E:324:VAL:HA	1.57	0.85
1:D:215:ARG:O	1:D:215:ARG:HD2	1.78	0.84
1:E:20:THR:HG22	1:E:22:GLY:H	1.43	0.84
1:F:340:THR:OG1	1:F:344:SER:CA	2.22	0.84
1:G:235:LEU:HB2	1:G:279:ILE:HD13	1.59	0.83
1:G:371:VAL:HG11	1:G:380:LEU:HG	1.57	0.83
1:E:235:LEU:HB2	1:E:279:ILE:HD13	1.60	0.83
1:H:20:THR:HG22	1:H:22:GLY:H	1.44	0.83
1:H:311:CYS:H	1:H:335:GLN:CG	1.87	0.82
1:G:337:TYR:OH	1:G:418:THR:CG2	2.26	0.82
1:A:248:THR:HG21	1:A:283:VAL:HG11	1.59	0.82
1:B:399:TYR:H	1:B:406:THR:HG22	1.42	0.82
1:A:399:TYR:H	1:A:406:THR:HG22	1.43	0.82
1:H:289:MET:HG2	1:H:316:LEU:HD11	1.60	0.82
1:H:286:PRO:HG3	1:H:314:SER:HB3	1.61	0.82
1:D:318:ARG:O	1:D:322:ASP:HB2	1.80	0.81
1:G:268:GLU:HA	1:G:271:LEU:HD23	1.62	0.81
1:B:400:HIS:O	1:B:402:ASN:N	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:THR:HG23	1:D:420:ASP:H	1.46	0.81
1:D:319:ASP:O	1:D:323:LYS:CG	2.26	0.81
1:G:370:LYS:HD2	1:G:415:TRP:CZ3	2.16	0.80
1:D:382:PRO:HG3	1:D:426:GLU:HB2	1.62	0.80
1:B:235:LEU:HB2	1:B:279:ILE:HD13	1.65	0.79
1:E:286:PRO:HG3	1:E:314:SER:HB2	1.64	0.79
1:G:74:VAL:HG13	1:G:120:PRO:HA	1.64	0.79
1:F:371:VAL:CG1	1:F:423:TYR:HD1	1.96	0.79
1:D:380:LEU:HD11	1:D:384:GLU:HG2	1.64	0.79
1:F:359:ALA:HB1	1:F:360:ILE:HA	1.63	0.79
1:G:294:LYS:HG2	1:G:295:SER:H	1.48	0.78
1:A:201:LEU:HD13	1:A:202:PRO:CD	2.14	0.78
1:B:83:ILE:HD13	1:B:261:MET:HE3	1.64	0.78
1:G:40:ILE:HG12	1:G:47:VAL:HG22	1.67	0.77
1:G:400:HIS:O	1:G:402:ASN:N	2.16	0.77
1:F:339:LEU:CD2	1:F:416:LEU:HD21	2.14	0.77
1:C:336:GLY:HA2	1:C:360:ILE:HG23	1.67	0.76
1:C:356:LYS:O	1:C:357:LYS:O	2.03	0.76
1:D:43:HIS:HE1	1:D:263:LYS:H	1.33	0.76
1:G:371:VAL:CG1	1:G:380:LEU:HB2	2.14	0.76
1:G:371:VAL:CG1	1:G:380:LEU:HG	2.16	0.76
1:D:235:LEU:HB2	1:D:279:ILE:HD13	1.68	0.76
1:G:371:VAL:CG1	1:G:380:LEU:CB	2.62	0.75
1:H:293:ALA:HB3	1:H:294:LYS:HD2	1.67	0.75
1:B:226:THR:HG23	1:B:228:ILE:H	1.48	0.75
1:E:284:VAL:HG12	1:E:288:ILE:HD11	1.68	0.75
1:B:347:ILE:HG12	1:B:364:MET:N	2.02	0.74
1:H:274:ILE:HA	1:H:279:ILE:HD12	1.69	0.74
1:G:159:GLU:HG2	1:G:163:SER:HB2	1.70	0.73
1:D:20:THR:HG22	1:D:22:GLY:H	1.53	0.73
1:E:112:ILE:HG23	1:E:140:LEU:HD21	1.69	0.73
1:H:235:LEU:HB2	1:H:279:ILE:HD13	1.71	0.73
1:F:122:LEU:HD13	1:F:145:LYS:HB3	1.71	0.73
1:H:423:TYR:H	1:H:423:TYR:HD1	1.32	0.73
1:H:286:PRO:HG2	1:H:287:PRO:HD3	1.69	0.73
1:A:336:GLY:HA2	1:A:348:LEU:HD11	1.71	0.72
1:C:353:ARG:CG	1:C:353:ARG:HH11	2.02	0.72
1:A:274:ILE:HG23	1:A:279:ILE:HG12	1.71	0.72
1:H:347:ILE:HG12	1:H:363:PRO:HA	1.71	0.72
1:B:59:ARG:NH2	1:B:170:ASP:O	2.23	0.72
1:G:300:GLU:O	1:G:302:ASN:ND2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:GLU:CG	1:D:297:LEU:HD22	2.20	0.71
1:F:16:VAL:HG12	1:F:217:VAL:HG21	1.72	0.71
1:H:201:LEU:HD22	1:H:202:PRO:HD2	1.72	0.71
1:B:264:LYS:HG3	1:B:265:PHE:H	1.56	0.71
1:C:266:GLU:HG2	1:C:269:PHE:H	1.56	0.71
1:F:340:THR:HA	1:F:344:SER:H	1.55	0.71
1:C:356:LYS:O	1:C:359:ALA:HB2	1.92	0.70
1:C:215:ARG:HH11	1:C:248:THR:HG22	1.57	0.69
1:C:347:ILE:CG2	1:C:361:GLY:HA3	2.22	0.69
1:B:274:ILE:HA	1:B:279:ILE:HD12	1.73	0.69
1:F:121:CYS:HB2	1:F:144:LYS:HE2	1.73	0.69
1:C:274:ILE:HG23	1:C:279:ILE:HG12	1.73	0.69
1:D:435:ARG:HB2	1:D:437:LYS:NZ	2.08	0.69
1:H:20:THR:HG22	1:H:22:GLY:N	2.08	0.69
1:E:20:THR:HG22	1:E:22:GLY:N	2.08	0.69
1:H:210:ARG:NH1	1:H:393:GLN:OE1	2.25	0.69
1:A:336:GLY:H	1:A:348:LEU:HG	1.57	0.69
1:E:122:LEU:HD13	1:E:145:LYS:HB3	1.75	0.69
1:F:425:ASP:O	1:F:426:GLU:CB	2.39	0.69
1:C:274:ILE:HG12	1:C:279:ILE:HD11	1.76	0.68
1:H:37:ASP:HA	1:H:47:VAL:CG1	2.23	0.68
1:B:39:ILE:HG23	1:B:259:ILE:HB	1.75	0.68
1:D:43:HIS:CE1	1:D:263:LYS:H	2.12	0.68
1:C:303:LEU:HD23	1:C:328:LEU:HD21	1.76	0.68
1:C:372:ILE:HD11	1:C:387:GLU:H	1.59	0.68
1:A:311:CYS:SG	1:A:312:GLY:N	2.67	0.68
1:G:369:VAL:HG22	1:G:390:PHE:CD1	2.29	0.67
1:A:335:GLN:HB3	1:A:348:LEU:HG	1.75	0.67
1:E:255:VAL:HG23	1:E:257:LEU:HG	1.76	0.67
1:E:346:LEU:HD21	1:E:395:LEU:HD21	1.76	0.67
1:C:20:THR:HG22	1:C:22:GLY:H	1.59	0.67
1:E:391:LYS:HB2	1:E:415:TRP:CD1	2.29	0.67
1:A:201:LEU:CD2	1:A:202:PRO:HD2	2.23	0.67
1:D:271:LEU:HD22	1:D:297:LEU:HD12	1.77	0.67
1:G:370:LYS:CD	1:G:415:TRP:CD2	2.78	0.67
1:C:195:SER:OG	1:C:196:SER:N	2.27	0.66
1:D:121:CYS:HB2	1:D:144:LYS:HE2	1.77	0.66
1:B:49:SER:N	1:B:52:GLN:OE1	2.21	0.66
1:H:37:ASP:HB3	1:H:40:ILE:HD11	1.77	0.66
1:B:376:THR:HG22	1:B:377:GLY:H	1.61	0.66
1:G:295:SER:O	1:G:295:SER:OG	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:LYS:O	1:C:359:ALA:CB	2.43	0.66
1:F:340:THR:HG1	1:F:344:SER:HA	1.56	0.66
1:G:421:LEU:HD23	1:G:422:GLY:N	2.11	0.66
1:H:274:ILE:HG23	1:H:279:ILE:HB	1.78	0.66
1:E:234:ILE:HD13	1:E:252:TYR:CE1	2.30	0.65
1:E:9:GLY:HA2	1:E:363:PRO:HG2	1.77	0.65
1:C:353:ARG:CB	1:C:353:ARG:HH11	2.08	0.65
1:E:282:ILE:HG22	1:E:284:VAL:HG13	1.78	0.65
1:C:237:ILE:HG23	1:C:262:VAL:HG23	1.77	0.65
1:E:40:ILE:HG12	1:E:47:VAL:HG23	1.79	0.65
1:D:40:ILE:HG12	1:D:47:VAL:HG23	1.79	0.65
1:E:286:PRO:HG3	1:E:314:SER:CB	2.27	0.65
1:B:347:ILE:N	1:B:364:MET:HB2	2.11	0.65
1:H:74:VAL:HG13	1:H:120:PRO:HA	1.79	0.65
1:G:327:ARG:HG2	1:G:328:LEU:HD13	1.79	0.64
1:C:122:LEU:HD13	1:C:145:LYS:HB3	1.79	0.64
1:H:148:VAL:HG21	1:H:155:ILE:HD12	1.78	0.64
1:C:353:ARG:HG2	1:C:353:ARG:HH11	1.62	0.64
1:C:284:VAL:HG12	1:C:289:MET:HG2	1.79	0.64
1:H:399:TYR:OH	1:H:405:ALA:HB3	1.98	0.64
1:A:266:GLU:HG3	1:A:267:GLY:H	1.62	0.64
1:D:295:SER:HG	1:D:297:LEU:HG	1.63	0.64
1:E:342:THR:HG21	1:E:396:MET:HB3	1.79	0.64
1:F:367:VAL:HA	1:F:392:SER:HB2	1.79	0.64
1:H:270:PHE:HE1	1:H:274:ILE:HD11	1.63	0.64
1:A:274:ILE:HG12	1:A:279:ILE:HD11	1.80	0.63
1:B:369:VAL:HG12	1:B:390:PHE:CE1	2.34	0.63
1:D:445:TYR:O	1:D:447:VAL:N	2.32	0.63
1:B:43:HIS:CE1	1:B:263:LYS:HG2	2.33	0.63
1:A:403:PRO:O	1:A:406:THR:HG23	1.98	0.63
1:D:20:THR:HG22	1:D:22:GLY:N	2.13	0.63
1:G:319:ASP:O	1:G:323:LYS:NZ	2.32	0.63
1:H:185:PRO:HB2	1:H:210:ARG:HG3	1.81	0.63
1:D:284:VAL:HG13	1:D:288:ILE:HB	1.79	0.63
1:F:159:GLU:HG2	1:F:163:SER:HB2	1.80	0.63
1:B:337:TYR:CE2	1:B:346:LEU:HB2	2.34	0.63
1:G:422:GLY:HA3	1:G:423:TYR:HB2	1.81	0.63
1:H:37:ASP:O	1:H:258:LYS:HG2	1.98	0.63
1:A:284:VAL:HG22	1:A:288:ILE:HD12	1.79	0.63
1:D:419:GLY:O	1:D:439:LEU:HB2	1.98	0.63
1:H:112:ILE:HG13	1:H:140:LEU:HD21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:NH2	1:A:170:ASP:O	2.32	0.63
1:G:75:VAL:HG12	1:G:122:LEU:HB3	1.80	0.63
1:F:376:THR:HG22	1:F:378:LYS:HZ2	1.63	0.62
1:D:374:ILE:HD12	1:D:374:ILE:H	1.64	0.62
1:H:59:ARG:NH2	1:H:170:ASP:O	2.33	0.62
1:A:286:PRO:HG2	1:A:287:PRO:HD3	1.80	0.62
1:G:224:TYR:HB3	1:G:348:LEU:HD12	1.80	0.62
1:C:284:VAL:HG13	1:C:288:ILE:HB	1.81	0.62
1:H:9:GLY:HA2	1:H:363:PRO:HG2	1.82	0.62
1:C:322:ASP:O	1:C:324:VAL:N	2.27	0.62
1:H:342:THR:HG22	1:H:396:MET:HB3	1.82	0.62
1:B:193:MET:O	1:B:205:VAL:N	2.27	0.61
1:D:384:GLU:HG3	1:D:385:LYS:H	1.65	0.61
1:H:330:VAL:O	1:H:332:GLY:N	2.33	0.61
1:B:122:LEU:HD13	1:B:145:LYS:HB3	1.82	0.61
1:D:224:TYR:HA	1:D:334:LEU:HD21	1.82	0.61
1:F:40:ILE:HG12	1:F:47:VAL:HG22	1.81	0.61
1:G:350:PRO:HB2	1:G:352:ASP:OD1	2.01	0.61
1:C:75:VAL:HG12	1:C:122:LEU:HB3	1.83	0.61
1:D:297:LEU:HD12	1:D:297:LEU:O	2.00	0.61
1:H:286:PRO:HG3	1:H:314:SER:CB	2.30	0.61
1:C:59:ARG:NH2	1:C:170:ASP:O	2.34	0.61
1:H:325:ALA:HB1	1:H:332:GLY:HA2	1.81	0.61
1:D:178:PHE:O	1:F:11:ARG:NH1	2.25	0.61
1:F:425:ASP:C	1:F:426:GLU:HG2	2.20	0.61
1:D:439:LEU:HD23	1:D:440:ILE:HB	1.83	0.61
1:E:270:PHE:HE1	1:E:274:ILE:HD11	1.66	0.61
1:D:438:GLU:OE1	1:D:439:LEU:N	2.34	0.61
1:F:371:VAL:HG12	1:F:423:TYR:HD1	1.64	0.61
1:D:429:PHE:HA	1:D:430:ILE:HB	1.83	0.61
1:G:286:PRO:HG3	1:G:314:SER:H	1.64	0.61
1:A:193:MET:HG3	1:A:207:ILE:HD12	1.82	0.60
1:E:74:VAL:HG12	1:E:120:PRO:HB3	1.82	0.60
1:G:274:ILE:HA	1:G:279:ILE:HD12	1.82	0.60
1:H:89:LEU:HD21	1:H:246:LEU:HD11	1.82	0.60
1:F:224:TYR:HA	1:F:334:LEU:HD21	1.82	0.60
1:F:274:ILE:HA	1:F:279:ILE:HD12	1.83	0.60
1:F:371:VAL:CG1	1:F:423:TYR:CD1	2.80	0.60
1:A:201:LEU:CD1	1:A:202:PRO:CD	2.76	0.60
1:B:224:TYR:CE1	1:B:348:LEU:O	2.55	0.60
1:F:39:ILE:HG23	1:F:259:ILE:HB	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:LEU:HD22	1:D:297:LEU:CD1	2.30	0.60
1:C:39:ILE:HG23	1:C:259:ILE:HB	1.82	0.60
1:G:274:ILE:HG23	1:G:279:ILE:HB	1.82	0.60
1:E:367:VAL:HA	1:E:392:SER:HB2	1.83	0.60
1:G:234:ILE:HD13	1:G:252:TYR:CE1	2.37	0.60
1:D:208:SER:HB3	1:D:397:LYS:HD2	1.82	0.60
1:B:74:VAL:HG13	1:B:120:PRO:HA	1.84	0.59
1:H:270:PHE:CE1	1:H:274:ILE:HD11	2.36	0.59
1:C:338:GLY:HA3	1:C:346:LEU:HB2	1.85	0.59
1:F:339:LEU:HD13	1:F:416:LEU:HD21	1.83	0.59
1:F:339:LEU:HD22	1:F:416:LEU:CD2	2.30	0.59
1:A:184:ASP:OD2	1:A:187:GLU:HG2	2.02	0.59
1:G:7:VAL:HG23	1:G:369:VAL:O	2.02	0.59
1:H:203:LYS:HB2	1:H:399:TYR:CE2	2.37	0.59
1:B:121:CYS:HB2	1:B:144:LYS:HE2	1.83	0.59
1:B:339:LEU:HB3	1:B:344:SER:HB3	1.83	0.59
1:D:119:LYS:HG2	1:D:142:PHE:CE2	2.38	0.59
1:D:268:GLU:HG3	1:D:297:LEU:HD22	1.85	0.59
1:B:342:THR:O	1:B:343:CYS:HB2	2.03	0.59
1:B:372:ILE:HD12	1:B:384:GLU:OE2	2.01	0.59
1:D:346:LEU:HD13	1:D:390:PHE:CD2	2.37	0.59
1:H:260:VAL:HG21	1:H:279:ILE:HD11	1.85	0.59
1:B:27:GLN:NE2	1:H:12:PRO:O	2.36	0.59
1:C:356:LYS:O	1:C:357:LYS:C	2.41	0.59
1:H:86:PHE:O	1:H:90:ILE:HG12	2.03	0.59
1:C:274:ILE:HG12	1:C:279:ILE:CD1	2.33	0.58
1:E:353:ARG:HB3	1:E:354:GLU:HA	1.84	0.58
1:H:196:SER:HB3	1:H:202:PRO:HA	1.85	0.58
1:F:307:THR:O	1:F:330:VAL:HG23	2.03	0.58
1:E:39:ILE:HG23	1:E:259:ILE:HB	1.85	0.58
1:E:55:GLU:OE2	1:E:59:ARG:NH1	2.36	0.58
1:H:215:ARG:HH21	1:H:248:THR:HA	1.68	0.58
1:D:284:VAL:CG1	1:D:288:ILE:HB	2.33	0.58
1:F:320:ILE:O	1:F:324:VAL:HG23	2.03	0.58
1:F:339:LEU:HD13	1:F:416:LEU:CD2	2.34	0.58
1:H:55:GLU:OE2	1:H:59:ARG:NH1	2.35	0.58
1:A:298:VAL:HB	1:A:327:ARG:HH21	1.67	0.58
1:G:266:GLU:OE2	1:G:288:ILE:HG12	2.03	0.58
1:B:224:TYR:HE1	1:B:348:LEU:O	1.86	0.58
1:G:300:GLU:O	1:G:302:ASN:N	2.37	0.58
1:A:186:LEU:O	1:A:397:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ILE:HD13	1:B:203:LYS:O	2.03	0.58
1:D:388:ILE:HG13	1:D:418:THR:HG21	1.85	0.58
1:F:7:VAL:HB	1:F:369:VAL:HG22	1.85	0.58
1:E:193:MET:O	1:E:205:VAL:N	2.30	0.57
1:E:282:ILE:HG12	1:E:306:LEU:HD11	1.85	0.57
1:F:315:PRO:O	1:F:317:GLY:N	2.37	0.57
1:F:189:THR:HG23	1:F:206:VAL:HG13	1.86	0.57
1:H:265:PHE:CD1	1:H:265:PHE:N	2.73	0.57
1:H:40:ILE:HG12	1:H:47:VAL:HG22	1.87	0.57
1:G:189:THR:HG23	1:G:206:VAL:HG13	1.87	0.57
1:C:337:TYR:CG	1:C:337:TYR:O	2.57	0.57
1:E:391:LYS:HB2	1:E:415:TRP:HD1	1.68	0.57
1:G:371:VAL:CG1	1:G:380:LEU:CG	2.70	0.57
1:H:340:THR:OG1	1:H:341:GLU:N	2.37	0.57
1:E:189:THR:HG23	1:E:206:VAL:HG23	1.86	0.57
1:H:95:GLN:HB2	1:H:97:ILE:HG12	1.86	0.57
1:A:89:LEU:HD21	1:A:246:LEU:HD11	1.87	0.57
1:B:255:VAL:HG23	1:B:257:LEU:HG	1.85	0.57
1:A:265:PHE:HA	1:A:266:GLU:HB3	1.87	0.57
1:E:193:MET:HE1	1:E:246:LEU:HD22	1.87	0.57
1:D:355:LEU:CD2	1:D:356:LYS:HE2	2.34	0.57
1:A:95:GLN:HB2	1:A:97:ILE:HG12	1.87	0.56
1:H:140:LEU:HD22	1:H:142:PHE:CZ	2.40	0.56
1:H:316:LEU:HD22	1:H:320:ILE:HD12	1.87	0.56
1:A:282:ILE:HD12	1:A:306:LEU:HD21	1.86	0.56
1:C:382:PRO:C	1:C:384:GLU:H	2.09	0.56
1:D:297:LEU:HD12	1:D:297:LEU:C	2.26	0.56
1:D:435:ARG:HB2	1:D:437:LYS:HZ2	1.67	0.56
1:E:292:LEU:HG	1:E:327:ARG:HH11	1.69	0.56
1:B:286:PRO:HG2	1:B:287:PRO:HD3	1.88	0.56
1:H:334:LEU:HB3	1:H:349:SER:HB3	1.86	0.56
1:D:338:GLY:HA3	1:D:346:LEU:HB2	1.86	0.56
1:E:275:GLN:O	1:E:303:LEU:HD21	2.06	0.56
1:D:95:GLN:HB2	1:D:97:ILE:HG12	1.88	0.56
1:B:371:VAL:HG21	1:B:385:LYS:HA	1.88	0.56
1:C:55:GLU:OE2	1:C:59:ARG:NH1	2.38	0.56
1:D:420:ASP:OD1	1:D:438:GLU:HA	2.05	0.56
1:F:16:VAL:HG13	1:F:366:TYR:CZ	2.41	0.56
1:H:399:TYR:H	1:H:406:THR:HG22	1.70	0.56
1:B:260:VAL:HG21	1:B:279:ILE:HD11	1.87	0.56
1:E:42:ALA:HB3	1:E:262:VAL:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:325:ALA:HB2	1:G:333:ILE:HG23	1.88	0.56
1:D:355:LEU:HD21	1:D:356:LYS:HE2	1.87	0.55
1:A:391:LYS:HG2	1:A:415:TRP:CD1	2.41	0.55
1:A:74:VAL:HG12	1:A:120:PRO:HB3	1.88	0.55
1:E:268:GLU:HG3	1:E:297:LEU:HG	1.87	0.55
1:H:337:TYR:CE2	1:H:339:LEU:CG	2.81	0.55
1:D:235:LEU:HB3	1:D:282:ILE:HG22	1.89	0.55
1:G:226:THR:HG22	1:G:228:ILE:H	1.71	0.55
1:E:117:ILE:O	1:E:118:SER:OG	2.24	0.55
1:E:320:ILE:HB	1:E:323:LYS:HG3	1.87	0.55
1:A:403:PRO:C	1:A:405:ALA:H	2.10	0.55
1:H:337:TYR:CZ	1:H:339:LEU:HA	2.42	0.55
1:D:369:VAL:HG22	1:D:390:PHE:CE1	2.41	0.55
1:B:234:ILE:HD13	1:B:252:TYR:CE1	2.41	0.55
1:C:322:ASP:O	1:C:324:VAL:HG22	2.06	0.55
1:D:429:PHE:CD2	1:F:177:LYS:HE2	2.42	0.55
1:F:195:SER:OG	1:F:196:SER:N	2.40	0.55
1:D:49:SER:N	1:D:52:GLN:OE1	2.26	0.54
1:H:17:PHE:O	1:H:213:THR:HG21	2.07	0.54
1:E:320:ILE:HD12	1:E:323:LYS:HD2	1.89	0.54
1:D:298:VAL:HB	1:D:327:ARG:HH21	1.72	0.54
1:E:347:ILE:HG12	1:E:363:PRO:HA	1.88	0.54
1:A:364:MET:O	1:A:367:VAL:HB	2.08	0.54
1:C:328:LEU:O	1:C:330:VAL:N	2.41	0.54
1:D:268:GLU:HG2	1:D:297:LEU:HD22	1.88	0.54
1:E:200:GLY:HA3	1:E:203:LYS:NZ	2.23	0.54
1:G:311:CYS:SG	1:G:312:GLY:N	2.81	0.54
1:G:376:THR:HG23	1:G:377:GLY:H	1.73	0.54
1:A:201:LEU:CG	1:A:202:PRO:CD	2.85	0.54
1:A:266:GLU:CG	1:A:267:GLY:H	2.20	0.54
1:D:5:ASN:OD1	1:D:5:ASN:N	2.40	0.54
1:C:162:PHE:HZ	1:D:152:MET:O	1.90	0.54
1:H:271:LEU:HD23	1:H:303:LEU:HD11	1.90	0.54
1:H:410:LEU:HD13	1:H:416:LEU:HG	1.88	0.54
1:A:234:ILE:HG13	1:A:281:SER:HB3	1.89	0.54
1:A:237:ILE:HG23	1:A:262:VAL:HG23	1.89	0.54
1:B:332:GLY:HA3	1:B:351:ASN:HB3	1.89	0.54
1:F:289:MET:HG2	1:F:324:VAL:HG21	1.88	0.54
1:F:339:LEU:CD1	1:F:416:LEU:HD21	2.38	0.54
1:G:371:VAL:HG11	1:G:380:LEU:CD1	2.38	0.54
1:B:270:PHE:HE2	1:B:288:ILE:CG2	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ASP:OD1	1:C:258:LYS:HE3	2.08	0.54
1:H:42:ALA:HB3	1:H:262:VAL:HG12	1.90	0.54
1:G:342:THR:HB	1:G:346:LEU:HD13	1.89	0.54
1:G:371:VAL:HG11	1:G:380:LEU:HB3	1.86	0.54
1:A:411:ASP:OD1	1:A:415:TRP:N	2.39	0.53
1:C:20:THR:HG22	1:C:22:GLY:N	2.23	0.53
1:F:74:VAL:HG22	1:F:98:PRO:HB2	1.90	0.53
1:H:119:LYS:HG2	1:H:142:PHE:CE2	2.43	0.53
1:H:186:LEU:HD13	1:H:210:ARG:NH2	2.22	0.53
1:A:201:LEU:HD22	1:A:202:PRO:HD3	0.63	0.53
1:C:334:LEU:HA	1:C:350:PRO:HG2	1.91	0.53
1:D:287:PRO:O	1:D:290:VAL:HG12	2.08	0.53
1:D:342:THR:HG22	1:D:396:MET:HB3	1.90	0.53
1:E:292:LEU:HD22	1:E:323:LYS:HB3	1.90	0.53
1:E:206:VAL:HG12	1:E:398:GLY:O	2.08	0.53
1:A:402:ASN:N	1:A:403:PRO:HD3	2.22	0.53
1:C:266:GLU:HG3	1:C:268:GLU:H	1.72	0.53
1:G:422:GLY:HA3	1:G:423:TYR:CB	2.39	0.53
1:C:40:ILE:HG12	1:C:47:VAL:HG22	1.89	0.53
1:D:424:TYR:HB3	1:D:432:VAL:HG23	1.90	0.53
1:E:349:SER:N	1:E:350:PRO:HD3	2.24	0.53
1:B:339:LEU:HD12	1:B:344:SER:O	2.08	0.53
1:E:67:TYR:HD2	1:E:69:LEU:HD13	1.72	0.53
1:F:285:PRO:HD2	1:F:288:ILE:HD12	1.89	0.53
1:G:235:LEU:HD12	1:G:260:VAL:O	2.09	0.53
1:C:9:GLY:HA2	1:C:363:PRO:HB2	1.90	0.53
1:D:403:PRO:HB2	1:D:405:ALA:H	1.74	0.53
1:D:9:GLY:HA2	1:D:363:PRO:HB2	1.91	0.53
1:E:287:PRO:O	1:E:290:VAL:HG22	2.09	0.53
1:G:39:ILE:HG23	1:G:259:ILE:HB	1.91	0.53
1:H:85:PHE:HE1	1:H:89:LEU:HD22	1.74	0.53
1:H:334:LEU:HD22	1:H:350:PRO:O	2.09	0.53
1:B:89:LEU:HD11	1:B:191:LEU:HD21	1.91	0.53
1:F:339:LEU:O	1:F:344:SER:O	2.27	0.53
1:C:89:LEU:HD11	1:C:191:LEU:HD21	1.91	0.52
1:D:214:ILE:O	1:D:217:VAL:HG13	2.10	0.52
1:D:268:GLU:HG3	1:D:297:LEU:CD2	2.39	0.52
1:E:293:ALA:H	1:E:327:ARG:HH11	1.56	0.52
1:G:266:GLU:CG	1:G:267:GLY:H	2.21	0.52
1:A:399:TYR:H	1:A:406:THR:CG2	2.18	0.52
1:B:285:PRO:HD2	1:B:288:ILE:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:VAL:HG12	1:E:122:LEU:HB3	1.91	0.52
1:G:374:ILE:HD12	1:G:374:ILE:H	1.73	0.52
1:A:403:PRO:O	1:A:405:ALA:N	2.41	0.52
1:D:319:ASP:HB3	1:D:323:LYS:HE3	1.92	0.52
1:E:270:PHE:O	1:E:273:THR:OG1	2.26	0.52
1:C:234:ILE:O	1:C:260:VAL:HG22	2.10	0.52
1:C:380:LEU:HD23	1:C:384:GLU:HB3	1.92	0.52
1:B:319:ASP:O	1:B:323:LYS:HG2	2.10	0.52
1:H:234:ILE:HG13	1:H:281:SER:HB3	1.90	0.52
1:H:402:ASN:O	1:H:406:THR:HG23	2.10	0.52
1:H:37:ASP:HA	1:H:47:VAL:HG11	1.90	0.52
1:A:336:GLY:H	1:A:348:LEU:CG	2.21	0.52
1:A:339:LEU:HB2	1:A:342:THR:HG23	1.91	0.52
1:C:287:PRO:O	1:C:290:VAL:HG12	2.10	0.52
1:D:43:HIS:CE1	1:D:262:VAL:HG13	2.45	0.52
1:A:37:ASP:HB3	1:A:40:ILE:HD11	1.91	0.52
1:B:112:ILE:HG23	1:B:140:LEU:HD21	1.92	0.52
1:C:210:ARG:NH1	1:C:393:GLN:OE1	2.42	0.52
1:D:307:THR:HG22	1:D:308:GLU:HG3	1.91	0.52
1:E:301:TYR:OH	1:E:304:SER:N	2.43	0.52
1:G:111:MET:HG3	1:G:115:LEU:HD22	1.92	0.52
1:A:328:LEU:HB2	1:A:330:VAL:HG12	1.91	0.52
1:D:268:GLU:OE2	1:D:268:GLU:N	2.43	0.52
1:D:405:ALA:HA	1:D:408:ASP:HB2	1.90	0.52
1:E:16:VAL:HG23	1:E:366:TYR:CZ	2.45	0.52
1:A:287:PRO:O	1:A:290:VAL:HG12	2.10	0.51
1:A:295:SER:O	1:A:298:VAL:HG23	2.10	0.51
1:B:269:PHE:HA	1:B:272:LYS:HD2	1.90	0.51
1:C:266:GLU:CG	1:C:269:PHE:H	2.22	0.51
1:D:318:ARG:O	1:D:322:ASP:CB	2.55	0.51
1:H:13:ARG:HD2	1:H:222:PRO:HD2	1.92	0.51
1:B:201:LEU:HG	1:B:202:PRO:HD2	1.91	0.51
1:C:353:ARG:HG2	1:C:353:ARG:NH1	2.21	0.51
1:E:26:TYR:HB2	1:E:94:TYR:CE1	2.46	0.51
1:H:337:TYR:O	1:H:339:LEU:HD12	2.10	0.51
1:B:411:ASP:OD2	1:B:415:TRP:HB2	2.11	0.51
1:H:405:ALA:HA	1:H:408:ASP:HB2	1.93	0.51
1:B:307:THR:O	1:B:330:VAL:HG23	2.10	0.51
1:C:356:LYS:C	1:C:357:LYS:O	2.48	0.51
1:D:342:THR:CG2	1:D:396:MET:HB3	2.41	0.51
1:G:285:PRO:HD2	1:G:288:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:LEU:HD11	1:H:191:LEU:HD21	1.90	0.51
1:C:399:TYR:H	1:C:406:THR:CG2	2.15	0.51
1:C:347:ILE:CG2	1:C:361:GLY:CA	2.89	0.51
1:C:6:ILE:HG12	1:C:380:LEU:O	2.10	0.51
1:F:382:PRO:HA	1:F:425:ASP:HB2	1.92	0.51
1:D:89:LEU:HD21	1:D:246:LEU:HD11	1.93	0.51
1:F:376:THR:CG2	1:F:378:LYS:NZ	2.74	0.51
1:G:42:ALA:HB3	1:G:262:VAL:HG12	1.93	0.51
1:A:32:TYR:O	1:A:33:SER:HB2	2.11	0.51
1:F:374:ILE:HG13	1:F:423:TYR:OH	2.11	0.51
1:B:127:LYS:HE3	1:B:150:ASP:O	2.10	0.51
1:H:395:LEU:HD13	1:H:416:LEU:HD12	1.93	0.51
1:A:306:LEU:HG	1:A:309:ILE:HD11	1.93	0.50
1:C:295:SER:O	1:C:298:VAL:HG22	2.12	0.50
1:E:349:SER:H	1:E:350:PRO:HD3	1.75	0.50
1:H:107:THR:HG23	1:H:110:GLU:OE1	2.11	0.50
1:C:308:GLU:HG2	1:C:331:HIS:HE1	1.76	0.50
1:C:67:TYR:HD2	1:C:69:LEU:HD13	1.75	0.50
1:E:285:PRO:HD2	1:E:288:ILE:CD1	2.42	0.50
1:F:9:GLY:HA2	1:F:363:PRO:HB2	1.93	0.50
1:G:278:LYS:HG3	1:G:305:SER:OG	2.11	0.50
1:B:265:PHE:CE1	1:B:288:ILE:HG12	2.46	0.50
1:F:71:HIS:HB3	1:F:188:ARG:NH1	2.26	0.50
1:G:119:LYS:HA	1:G:142:PHE:CE2	2.46	0.50
1:C:121:CYS:HB2	1:C:144:LYS:HE2	1.94	0.50
1:H:306:LEU:HG	1:H:309:ILE:HD11	1.94	0.50
1:C:215:ARG:HH12	1:C:248:THR:HG22	1.76	0.50
1:D:320:ILE:O	1:D:324:VAL:HG13	2.11	0.50
1:E:338:GLY:O	1:E:345:ALA:HA	2.11	0.50
1:G:197:GLY:C	1:G:199:THR:H	2.14	0.50
1:F:369:VAL:HG12	1:F:390:PHE:CE1	2.47	0.50
1:C:130:LEU:HB3	1:C:131:PRO:HD3	1.94	0.50
1:F:112:ILE:HG23	1:F:140:LEU:HD21	1.93	0.50
1:G:375:ASN:OD1	1:G:375:ASN:N	2.43	0.49
1:B:371:VAL:HA	1:B:387:GLU:O	2.12	0.49
1:B:387:GLU:H	1:B:387:GLU:CD	2.15	0.49
1:E:206:VAL:HG13	1:E:397:LYS:HB2	1.94	0.49
1:F:75:VAL:HG12	1:F:122:LEU:HB3	1.93	0.49
1:H:184:ASP:OD2	1:H:187:GLU:HG2	2.13	0.49
1:C:382:PRO:O	1:C:384:GLU:N	2.36	0.49
1:D:226:THR:O	1:D:228:ILE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:THR:HG22	1:F:308:GLU:HG3	1.94	0.49
1:D:306:LEU:HG	1:D:309:ILE:HD11	1.94	0.49
1:H:287:PRO:O	1:H:290:VAL:HG22	2.12	0.49
1:H:334:LEU:HB3	1:H:349:SER:CB	2.41	0.49
1:D:369:VAL:HA	1:D:389:CYS:O	2.12	0.49
1:F:346:LEU:HD12	1:F:390:PHE:CD2	2.48	0.49
1:B:270:PHE:O	1:B:271:LEU:HG	2.12	0.49
1:A:270:PHE:O	1:A:274:ILE:HG13	2.13	0.49
1:D:159:GLU:HG2	1:D:163:SER:HB2	1.94	0.49
1:D:221:ASP:OD1	1:D:223:ILE:N	2.37	0.49
1:G:367:VAL:HA	1:G:392:SER:HB2	1.94	0.49
1:H:107:THR:HG1	1:H:109:ARG:HG3	1.78	0.49
1:C:402:ASN:O	1:C:406:THR:HG23	2.12	0.48
1:E:49:SER:N	1:E:52:GLN:OE1	2.27	0.48
1:C:207:ILE:HD13	1:C:247:PHE:HZ	1.77	0.48
1:D:270:PHE:CE1	1:D:274:ILE:HD11	2.48	0.48
1:F:376:THR:HG22	1:F:378:LYS:NZ	2.26	0.48
1:A:32:TYR:C	1:A:34:TYR:H	2.16	0.48
1:D:284:VAL:HG22	1:D:288:ILE:HD12	1.95	0.48
1:D:302:ASN:OD1	1:D:304:SER:HB2	2.14	0.48
1:D:424:TYR:HD2	1:D:430:ILE:HD11	1.78	0.48
1:H:330:VAL:C	1:H:332:GLY:H	2.16	0.48
1:H:364:MET:O	1:H:367:VAL:HB	2.13	0.48
1:A:270:PHE:CE2	1:A:274:ILE:HD11	2.47	0.48
1:C:71:HIS:HB3	1:C:188:ARG:NH1	2.28	0.48
1:H:334:LEU:C	1:H:349:SER:HB2	2.33	0.48
1:B:285:PRO:HD2	1:B:288:ILE:HD12	1.94	0.48
1:A:413:ASP:OD1	1:A:413:ASP:N	2.47	0.48
1:G:112:ILE:HG23	1:G:140:LEU:HD21	1.96	0.48
1:H:107:THR:OG1	1:H:109:ARG:HG3	2.13	0.48
1:B:59:ARG:NH2	1:B:173:PHE:HB3	2.29	0.48
1:B:369:VAL:HG12	1:B:390:PHE:HE1	1.78	0.48
1:C:308:GLU:HG2	1:C:331:HIS:CE1	2.48	0.48
1:C:6:ILE:HG23	1:C:381:GLY:HA2	1.96	0.48
1:B:309:ILE:HG12	1:B:330:VAL:HG21	1.94	0.48
1:C:380:LEU:HB3	1:C:382:PRO:HD2	1.95	0.48
1:E:13:ARG:HD3	1:E:222:PRO:HD2	1.94	0.48
1:H:108:GLU:O	1:H:112:ILE:HG22	2.13	0.48
1:A:59:ARG:NH2	1:A:173:PHE:HB3	2.29	0.47
1:F:234:ILE:HD13	1:F:252:TYR:CE1	2.48	0.47
1:F:89:LEU:HD11	1:F:191:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:LEU:HD13	1:H:90:ILE:HD12	1.95	0.47
1:B:373:ASP:HB3	1:B:376:THR:HB	1.96	0.47
1:D:418:THR:HG23	1:D:420:ASP:N	2.23	0.47
1:C:193:MET:HG3	1:C:207:ILE:HD12	1.95	0.47
1:G:197:GLY:O	1:G:199:THR:N	2.47	0.47
1:G:13:ARG:HD2	1:G:222:PRO:HD2	1.95	0.47
1:D:418:THR:HG23	1:D:419:GLY:N	2.30	0.47
1:G:294:LYS:HB3	1:G:296:PRO:HD3	1.95	0.47
1:A:342:THR:O	1:A:344:SER:N	2.47	0.47
1:G:282:ILE:HG12	1:G:306:LEU:HD11	1.97	0.47
1:G:396:MET:HG3	1:G:398:GLY:H	1.78	0.47
1:C:380:LEU:CD2	1:C:384:GLU:HB3	2.45	0.47
1:E:335:GLN:H	1:E:350:PRO:CG	2.28	0.47
1:F:223:ILE:HG23	1:F:350:PRO:HB3	1.97	0.47
1:H:228:ILE:HG13	1:H:232:THR:OG1	2.15	0.47
1:C:364:MET:O	1:C:367:VAL:HB	2.15	0.47
1:D:69:LEU:HD11	1:D:122:LEU:HD13	1.95	0.47
1:E:309:ILE:HG12	1:E:330:VAL:HG21	1.97	0.47
1:F:89:LEU:HD13	1:F:99:MET:HG2	1.96	0.47
1:B:295:SER:OG	1:B:298:VAL:HB	2.14	0.47
1:D:205:VAL:HG13	1:D:396:MET:CE	2.45	0.47
1:D:274:ILE:HA	1:D:279:ILE:HD12	1.97	0.47
1:H:150:ASP:N	1:H:150:ASP:OD1	2.47	0.47
1:H:303:LEU:HD22	1:H:328:LEU:CD2	2.45	0.47
1:A:107:THR:HG23	1:A:110:GLU:CD	2.35	0.47
1:C:306:LEU:HD23	1:C:328:LEU:CD2	2.44	0.47
1:E:327:ARG:O	1:E:329:LYS:N	2.47	0.47
1:D:307:THR:O	1:D:330:VAL:HG23	2.15	0.47
1:D:347:ILE:HG12	1:D:363:PRO:HA	1.96	0.47
1:E:342:THR:CG2	1:E:396:MET:HB3	2.44	0.47
1:H:426:GLU:HA	1:H:427:ASP:HA	1.64	0.47
1:A:345:ALA:C	1:A:346:LEU:HD12	2.35	0.47
1:E:263:LYS:HE2	1:E:263:LYS:HB2	1.68	0.47
1:F:250:LEU:HD23	1:F:250:LEU:HA	1.47	0.47
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.71	0.46
1:D:273:THR:HG22	1:D:277:TYR:HE2	1.79	0.46
1:E:307:THR:O	1:E:330:VAL:HG22	2.15	0.46
1:E:402:ASN:O	1:E:406:THR:HG23	2.14	0.46
1:B:191:LEU:HD22	1:B:193:MET:HE2	1.97	0.46
1:B:268:GLU:O	1:B:272:LYS:HG3	2.16	0.46
1:H:270:PHE:CD2	1:H:288:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ILE:HD11	1:C:224:TYR:CZ	2.50	0.46
1:G:275:GLN:CG	1:G:300:GLU:HB3	2.46	0.46
1:H:341:GLU:OE1	1:H:341:GLU:N	2.44	0.46
1:A:24:GLN:NE2	1:A:216:PHE:HD2	2.13	0.46
1:A:407:ARG:HA	1:A:407:ARG:HD3	1.63	0.46
1:E:59:ARG:NH2	1:E:170:ASP:O	2.49	0.46
1:E:74:VAL:HG22	1:E:98:PRO:HB2	1.97	0.46
1:E:20:THR:HG23	1:E:209:HIS:ND1	2.30	0.46
1:E:343:CYS:HB2	1:E:346:LEU:HD11	1.96	0.46
1:F:353:ARG:HB3	1:F:354:GLU:H	1.57	0.46
1:F:356:LYS:HB3	1:F:357:LYS:HB2	1.97	0.46
1:H:399:TYR:CE2	1:H:402:ASN:HB3	2.49	0.46
1:A:15:LEU:HD23	1:A:15:LEU:HA	1.69	0.46
1:C:7:VAL:HB	1:C:369:VAL:O	2.15	0.46
1:D:318:ARG:O	1:D:322:ASP:OD2	2.33	0.46
1:D:29:LEU:HD23	1:D:54:PHE:HA	1.98	0.46
1:F:319:ASP:HB3	1:F:322:ASP:HB3	1.96	0.46
1:G:237:ILE:HG13	1:G:262:VAL:HG23	1.98	0.46
1:H:234:ILE:HD13	1:H:252:TYR:CE1	2.50	0.46
1:H:340:THR:C	1:H:342:THR:H	2.18	0.46
1:B:306:LEU:HD12	1:B:306:LEU:HA	1.67	0.46
1:C:300:GLU:HG3	1:F:329:LYS:HD3	1.98	0.46
1:H:191:LEU:HD22	1:H:193:MET:HE2	1.98	0.46
1:H:198:THR:C	1:H:199:THR:HG1	2.17	0.46
1:D:316:LEU:O	1:D:320:ILE:HD12	2.15	0.46
1:E:315:PRO:HB2	1:E:319:ASP:OD2	2.16	0.46
1:F:226:THR:HG22	1:F:228:ILE:H	1.80	0.46
1:A:174:ASP:OD2	1:A:177:LYS:NZ	2.47	0.46
1:A:32:TYR:O	1:A:34:TYR:N	2.47	0.46
1:D:250:LEU:HA	1:D:250:LEU:HD23	1.63	0.46
1:E:349:SER:N	1:E:350:PRO:CD	2.79	0.46
1:F:275:GLN:HE22	1:F:301:TYR:HD2	1.64	0.46
1:D:345:ALA:HB1	1:D:348:LEU:HD11	1.98	0.46
1:G:342:THR:HB	1:G:346:LEU:CD1	2.46	0.46
1:F:270:PHE:O	1:F:274:ILE:HG13	2.15	0.45
1:G:345:ALA:C	1:G:346:LEU:HD12	2.37	0.45
1:H:103:ASN:HB3	1:H:106:TYR:CD1	2.50	0.45
1:H:334:LEU:HD21	1:H:355:LEU:HG	1.98	0.45
1:B:315:PRO:O	1:B:317:GLY:N	2.49	0.45
1:D:397:LYS:HZ2	1:D:397:LYS:HB3	1.81	0.45
1:D:421:LEU:HD23	1:D:438:GLU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:325:ALA:CB	1:H:332:GLY:HA2	2.47	0.45
1:H:311:CYS:O	1:H:335:GLN:HB3	2.16	0.45
1:B:117:ILE:HG21	1:B:203:LYS:O	2.16	0.45
1:B:215:ARG:HH21	1:B:248:THR:HG22	1.81	0.45
1:C:48:ILE:HD12	1:C:52:GLN:NE2	2.32	0.45
1:F:284:VAL:HB	1:F:288:ILE:HB	1.97	0.45
1:G:378:LYS:HB2	1:G:378:LYS:HE2	1.66	0.45
1:H:184:ASP:OD2	1:H:186:LEU:HB3	2.16	0.45
1:A:75:VAL:HG12	1:A:122:LEU:HB3	1.98	0.45
1:E:237:ILE:CD1	1:E:262:VAL:HG23	2.34	0.45
1:H:250:LEU:HD12	1:H:250:LEU:HA	1.76	0.45
1:A:127:LYS:HG3	1:A:150:ASP:OD1	2.17	0.45
1:C:286:PRO:HB2	1:C:287:PRO:HD3	1.99	0.45
1:D:85:PHE:HE1	1:D:89:LEU:HD22	1.81	0.45
1:A:20:THR:HA	1:A:185:PRO:HB3	1.98	0.45
1:B:400:HIS:CG	1:B:401:ASN:H	2.34	0.45
1:D:339:LEU:HD22	1:D:340:THR:H	1.82	0.45
1:F:7:VAL:HB	1:F:369:VAL:CG2	2.47	0.45
1:G:250:LEU:HD12	1:G:250:LEU:HA	1.55	0.45
1:A:12:PRO:O	1:A:13:ARG:HB2	2.16	0.45
1:A:265:PHE:HB2	1:A:266:GLU:OE2	2.16	0.45
1:D:270:PHE:O	1:D:274:ILE:HG13	2.16	0.45
1:H:267:GLY:O	1:H:270:PHE:HB3	2.17	0.45
1:D:201:LEU:HD12	1:D:202:PRO:HD2	1.98	0.45
1:E:327:ARG:C	1:E:329:LYS:H	2.20	0.45
1:F:107:THR:HG22	1:F:110:GLU:HG3	1.99	0.45
1:G:349:SER:HA	1:G:350:PRO:HD3	1.59	0.45
1:H:360:ILE:HG12	1:H:423:TYR:CE2	2.52	0.45
1:D:272:LYS:HZ3	1:E:331:HIS:CD2	2.34	0.45
1:E:191:LEU:HD13	1:E:193:MET:CE	2.47	0.45
1:G:339:LEU:CD1	1:G:341:GLU:HB2	2.47	0.45
1:H:210:ARG:HH22	1:H:393:GLN:CD	2.20	0.45
1:D:17:PHE:HA	1:D:18:PRO:HD3	1.82	0.45
1:D:421:LEU:HG	1:D:437:LYS:HE2	1.99	0.45
1:E:326:LYS:HA	1:E:326:LYS:HD3	1.61	0.45
1:H:397:LYS:HD3	1:H:397:LYS:HA	1.73	0.45
1:A:274:ILE:HG12	1:A:279:ILE:CD1	2.45	0.44
1:C:284:VAL:CG1	1:C:288:ILE:HB	2.46	0.44
1:E:89:LEU:HD11	1:E:191:LEU:HD21	1.99	0.44
1:F:211:SER:O	1:F:215:ARG:HG3	2.17	0.44
1:F:425:ASP:O	1:F:426:GLU:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:GLU:O	1:G:270:PHE:N	2.42	0.44
1:H:59:ARG:NH2	1:H:173:PHE:HB3	2.32	0.44
1:B:89:LEU:CD1	1:B:99:MET:HG2	2.47	0.44
1:G:372:ILE:O	1:G:373:ASP:C	2.56	0.44
1:A:171:HIS:CD2	1:H:155:ILE:HA	2.52	0.44
1:B:300:GLU:HG2	1:C:329:LYS:NZ	2.33	0.44
1:E:250:LEU:HD12	1:E:250:LEU:HA	1.55	0.44
1:E:282:ILE:CG1	1:E:306:LEU:HD11	2.47	0.44
1:F:194:THR:HG23	1:F:203:LYS:O	2.17	0.44
1:F:315:PRO:HB2	1:F:320:ILE:HD12	1.98	0.44
1:A:341:GLU:OE1	1:A:341:GLU:N	2.49	0.44
1:E:292:LEU:CD2	1:E:323:LYS:HB3	2.48	0.44
1:F:285:PRO:HD2	1:F:288:ILE:CD1	2.48	0.44
1:F:295:SER:OG	1:F:297:LEU:HB2	2.17	0.44
1:G:67:TYR:HD2	1:G:69:LEU:HD13	1.81	0.44
1:H:204:GLY:O	1:H:400:HIS:N	2.37	0.44
1:H:211:SER:HB3	1:H:343:CYS:SG	2.58	0.44
1:H:282:ILE:HG22	1:H:284:VAL:HG22	1.99	0.44
1:A:324:VAL:HG23	1:A:333:ILE:HD11	2.00	0.44
1:B:44:THR:HG23	1:B:46:GLU:H	1.83	0.44
1:C:214:ILE:O	1:C:217:VAL:HB	2.18	0.44
1:D:308:GLU:O	1:D:309:ILE:HD13	2.18	0.44
1:D:397:LYS:NZ	1:D:397:LYS:HB3	2.33	0.44
1:F:207:ILE:HD11	1:F:342:THR:HG21	1.99	0.44
1:F:215:ARG:NH1	1:F:342:THR:O	2.43	0.44
1:H:37:ASP:CB	1:H:258:LYS:HE2	2.48	0.44
1:A:401:ASN:OD1	1:A:402:ASN:N	2.45	0.44
1:C:356:LYS:O	1:C:359:ALA:HB3	2.18	0.44
1:D:7:VAL:HB	1:D:430:ILE:HG12	1.98	0.44
1:E:71:HIS:HB3	1:E:188:ARG:NH1	2.33	0.44
1:E:253:PHE:HB2	1:E:254:PRO:HD3	2.00	0.44
1:G:380:LEU:HD22	1:G:380:LEU:HA	1.73	0.44
1:A:82:ASN:ND2	1:A:150:ASP:OD2	2.50	0.44
1:A:274:ILE:HG23	1:A:279:ILE:CG1	2.43	0.44
1:A:284:VAL:HG13	1:A:288:ILE:HB	2.00	0.44
1:C:271:LEU:HB3	1:C:301:TYR:CD2	2.53	0.44
1:D:71:HIS:HB3	1:D:188:ARG:NH1	2.32	0.44
1:G:120:PRO:HD2	1:G:142:PHE:HE2	1.83	0.44
1:G:285:PRO:HB2	1:G:287:PRO:HD2	2.00	0.44
1:B:270:PHE:O	1:B:270:PHE:CG	2.70	0.44
1:B:339:LEU:HB3	1:B:344:SER:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:PRO:O	1:C:13:ARG:HB2	2.18	0.44
1:C:282:ILE:HG23	1:C:306:LEU:HD11	2.00	0.44
1:C:365:PRO:O	1:C:366:TYR:HB2	2.18	0.44
1:H:293:ALA:HA	1:H:327:ARG:HD3	2.00	0.44
1:A:111:MET:HG3	1:A:115:LEU:HD22	2.00	0.43
1:E:285:PRO:HB2	1:E:287:PRO:HD2	1.99	0.43
1:E:302:ASN:C	1:E:303:LEU:HD12	2.38	0.43
1:F:371:VAL:HG11	1:F:423:TYR:HD1	1.77	0.43
1:G:193:MET:HE1	1:G:243:ALA:HA	2.00	0.43
1:H:15:LEU:HD23	1:H:15:LEU:HA	1.81	0.43
1:C:207:ILE:HD13	1:C:247:PHE:CZ	2.53	0.43
1:C:89:LEU:HD21	1:C:246:LEU:HD11	2.00	0.43
1:D:411:ASP:HB2	1:D:415:TRP:H	1.83	0.43
1:E:16:VAL:HG23	1:E:366:TYR:CE2	2.53	0.43
1:F:233:SER:HA	1:F:258:LYS:HB2	2.00	0.43
1:G:287:PRO:O	1:G:290:VAL:HG22	2.17	0.43
1:A:155:ILE:HA	1:H:171:HIS:CD2	2.53	0.43
1:A:365:PRO:O	1:A:366:TYR:HB2	2.17	0.43
1:B:289:MET:CE	1:B:311:CYS:HB3	2.49	0.43
1:D:339:LEU:HD22	1:D:340:THR:N	2.34	0.43
1:A:284:VAL:CG1	1:A:288:ILE:HB	2.49	0.43
1:B:211:SER:HA	1:B:394:MET:HA	2.01	0.43
1:D:108:GLU:HG3	1:D:136:VAL:HG22	1.99	0.43
1:E:264:LYS:HD2	1:E:264:LYS:HA	1.86	0.43
1:F:107:THR:CG2	1:F:110:GLU:H	2.32	0.43
1:A:401:ASN:C	1:A:403:PRO:HD3	2.39	0.43
1:A:58:CYS:O	1:A:62:VAL:HG23	2.19	0.43
1:B:122:LEU:HD12	1:B:123:MET:H	1.82	0.43
1:B:289:MET:HE1	1:B:311:CYS:HB3	2.01	0.43
1:C:239:PRO:HB3	1:C:241:HIS:NE2	2.33	0.43
1:C:306:LEU:HD12	1:C:306:LEU:HA	1.84	0.43
1:F:231:ASP:OD1	1:F:258:LYS:HE3	2.18	0.43
1:A:152:MET:O	1:H:162:PHE:HZ	2.02	0.43
1:A:337:TYR:O	1:A:345:ALA:HA	2.19	0.43
1:B:41:ASP:HB3	1:B:44:THR:HG22	1.99	0.43
1:C:15:LEU:HD23	1:C:15:LEU:HA	1.81	0.43
1:D:7:VAL:HG13	1:D:369:VAL:O	2.18	0.43
1:E:114:HIS:ND1	1:E:194:THR:HG21	2.34	0.43
1:H:286:PRO:CG	1:H:287:PRO:HD3	2.45	0.43
1:B:270:PHE:HE2	1:B:288:ILE:HG23	1.82	0.43
1:E:200:GLY:HA3	1:E:203:LYS:HZ1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:343:CYS:O	1:F:344:SER:OG	2.32	0.43
1:H:210:ARG:HB3	1:H:210:ARG:CZ	2.49	0.43
1:H:303:LEU:HD22	1:H:328:LEU:HD22	1.99	0.43
1:A:391:LYS:HE3	1:A:391:LYS:HB3	1.85	0.43
1:A:62:VAL:HG21	1:A:173:PHE:HE2	1.83	0.43
1:D:210:ARG:HG2	1:D:393:GLN:HB3	2.01	0.43
1:E:268:GLU:OE2	1:E:268:GLU:HA	2.18	0.43
1:E:281:SER:O	1:E:282:ILE:HD13	2.19	0.43
1:E:335:GLN:H	1:E:350:PRO:HG2	1.84	0.43
1:G:234:ILE:HD13	1:G:252:TYR:CZ	2.54	0.43
1:A:342:THR:HB	1:A:346:LEU:CD1	2.49	0.43
1:A:391:LYS:HG2	1:A:415:TRP:HA	2.01	0.43
1:B:140:LEU:HB3	1:B:142:PHE:CE2	2.54	0.43
1:B:391:LYS:HB2	1:B:415:TRP:CE3	2.53	0.43
1:C:17:PHE:HZ	1:C:23:LEU:HD22	1.84	0.43
1:E:210:ARG:O	1:E:214:ILE:HG13	2.19	0.43
1:E:289:MET:C	1:E:291:TYR:H	2.21	0.43
1:E:318:ARG:O	1:E:318:ARG:HG3	2.18	0.43
1:A:114:HIS:CE1	1:A:194:THR:HG1	2.36	0.43
1:B:150:ASP:N	1:B:150:ASP:OD1	2.52	0.43
1:B:234:ILE:HG13	1:B:281:SER:O	2.18	0.43
1:E:211:SER:O	1:E:215:ARG:HG3	2.18	0.43
1:E:293:ALA:H	1:E:327:ARG:NH1	2.17	0.43
1:F:223:ILE:CG2	1:F:350:PRO:HB3	2.48	0.43
1:G:341:GLU:N	1:G:341:GLU:OE1	2.50	0.43
1:A:121:CYS:HB2	1:A:144:LYS:HE2	2.00	0.42
1:A:266:GLU:OE2	1:A:288:ILE:HG12	2.18	0.42
1:C:340:THR:HG22	1:C:341:GLU:N	2.34	0.42
1:C:346:LEU:O	1:C:347:ILE:HG13	2.18	0.42
1:D:382:PRO:HB2	1:D:383:ARG:HD3	2.01	0.42
1:E:103:ASN:HB3	1:E:106:TYR:CE1	2.54	0.42
1:F:279:ILE:O	1:F:306:LEU:HD23	2.19	0.42
1:F:340:THR:O	1:F:340:THR:HG22	2.19	0.42
1:H:404:GLN:HG3	1:H:405:ALA:N	2.34	0.42
1:H:48:ILE:HA	1:H:52:GLN:OE1	2.19	0.42
1:B:191:LEU:HD13	1:B:193:MET:CE	2.49	0.42
1:C:353:ARG:HG3	1:C:354:GLU:N	2.34	0.42
1:C:372:ILE:HG13	1:C:387:GLU:O	2.20	0.42
1:D:383:ARG:HD3	1:D:383:ARG:N	2.35	0.42
1:G:130:LEU:HD11	1:G:158:VAL:HG11	2.00	0.42
1:G:306:LEU:HD12	1:G:306:LEU:HA	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:339:LEU:HD12	1:G:341:GLU:HB2	2.01	0.42
1:A:116:ASN:O	1:A:119:LYS:NZ	2.50	0.42
1:C:42:ALA:HB3	1:C:262:VAL:HG12	2.00	0.42
1:D:362:THR:HA	1:D:363:PRO:HD3	1.86	0.42
1:E:20:THR:CG2	1:E:22:GLY:H	2.24	0.42
1:E:314:SER:H	1:E:315:PRO:CD	2.31	0.42
1:E:388:ILE:O	1:E:418:THR:HG22	2.19	0.42
1:F:214:ILE:O	1:F:217:VAL:HB	2.19	0.42
1:G:77:ILE:HA	1:G:124:PHE:O	2.19	0.42
1:H:236:ALA:HB2	1:H:252:TYR:HE2	1.84	0.42
1:A:239:PRO:HB3	1:A:241:HIS:NE2	2.35	0.42
1:C:307:THR:HG22	1:C:308:GLU:HG3	2.01	0.42
1:E:301:TYR:CE1	1:E:303:LEU:HB2	2.54	0.42
1:G:203:LYS:HE2	1:G:399:TYR:CE1	2.54	0.42
1:H:290:VAL:HG12	1:H:320:ILE:HD13	2.01	0.42
1:H:344:SER:OG	1:H:345:ALA:N	2.49	0.42
1:B:386:GLY:C	1:B:421:LEU:HG	2.39	0.42
1:C:89:LEU:CD1	1:C:99:MET:HG2	2.48	0.42
1:D:215:ARG:C	1:D:215:ARG:HD2	2.35	0.42
1:E:208:SER:O	1:E:211:SER:OG	2.35	0.42
1:E:265:PHE:CD2	1:E:288:ILE:HG22	2.54	0.42
1:G:280:ALA:HA	1:G:305:SER:O	2.20	0.42
1:G:369:VAL:HG12	1:G:370:LYS:N	2.34	0.42
1:C:119:LYS:HG2	1:C:142:PHE:CE2	2.54	0.42
1:D:355:LEU:HD22	1:D:431:TYR:CZ	2.55	0.42
1:D:441:LYS:HG2	1:D:444:GLY:HA3	2.00	0.42
1:B:27:GLN:HG3	1:H:13:ARG:O	2.20	0.42
1:H:413:ASP:N	1:H:415:TRP:HD1	2.17	0.42
1:B:375:ASN:N	1:B:375:ASN:OD1	2.46	0.42
1:C:347:ILE:HG21	1:C:361:GLY:CA	2.49	0.42
1:D:266:GLU:HB3	1:D:267:GLY:H	1.49	0.42
1:E:150:ASP:OD1	1:E:150:ASP:N	2.45	0.42
1:E:316:LEU:O	1:E:316:LEU:HD12	2.20	0.42
1:F:290:VAL:HG12	1:F:320:ILE:HG21	2.02	0.42
1:G:365:PRO:O	1:G:366:TYR:HB2	2.20	0.42
1:B:284:VAL:HB	1:B:288:ILE:HB	2.01	0.42
1:C:115:LEU:HA	1:C:115:LEU:HD23	1.88	0.42
1:C:406:THR:O	1:C:410:LEU:N	2.27	0.42
1:E:270:PHE:CE1	1:E:274:ILE:HD11	2.50	0.42
1:E:306:LEU:HA	1:E:306:LEU:HD12	1.69	0.42
1:E:354:GLU:O	1:E:356:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:TYR:CE2	1:F:11:ARG:HG2	2.54	0.42
1:F:418:THR:OG1	1:F:420:ASP:O	2.38	0.42
1:B:191:LEU:HD13	1:B:193:MET:HE3	2.00	0.42
1:B:224:TYR:HD1	1:B:348:LEU:HD12	1.84	0.42
1:C:150:ASP:N	1:C:150:ASP:OD1	2.48	0.42
1:D:150:ASP:OD1	1:D:150:ASP:N	2.48	0.42
1:D:41:ASP:OD2	1:D:263:LYS:NZ	2.47	0.42
1:F:350:PRO:HB2	1:F:351:ASN:H	1.43	0.42
1:G:55:GLU:O	1:G:59:ARG:HG3	2.20	0.42
1:H:306:LEU:CD2	1:H:309:ILE:HD11	2.50	0.42
1:H:323:LYS:HB3	1:H:323:LYS:HE3	1.85	0.42
1:H:330:VAL:C	1:H:332:GLY:N	2.73	0.42
1:A:315:PRO:O	1:A:317:GLY:N	2.53	0.42
1:B:328:LEU:O	1:B:330:VAL:HG12	2.20	0.42
1:C:234:ILE:HG13	1:C:281:SER:HB3	2.02	0.42
1:D:130:LEU:HD11	1:D:158:VAL:HG11	2.01	0.42
1:D:234:ILE:HD13	1:D:252:TYR:CE1	2.55	0.42
1:D:320:ILE:O	1:D:322:ASP:N	2.51	0.42
1:D:439:LEU:HD23	1:D:440:ILE:CB	2.50	0.42
1:G:285:PRO:HD2	1:G:288:ILE:CD1	2.50	0.42
1:C:274:ILE:HG23	1:C:279:ILE:CG1	2.45	0.41
1:C:367:VAL:HA	1:C:392:SER:HB2	2.02	0.41
1:D:265:PHE:CD2	1:D:266:GLU:HB2	2.55	0.41
1:E:278:LYS:HG2	1:E:303:LEU:HD23	2.01	0.41
1:E:418:THR:HG23	1:E:420:ASP:H	1.85	0.41
1:F:359:ALA:CB	1:F:360:ILE:HA	2.42	0.41
1:H:298:VAL:HB	1:H:327:ARG:HH21	1.85	0.41
1:A:309:ILE:HD13	1:A:330:VAL:HG11	2.02	0.41
1:A:338:GLY:O	1:A:339:LEU:HD23	2.20	0.41
1:B:114:HIS:ND1	1:B:194:THR:HG21	2.34	0.41
1:B:193:MET:HE1	1:B:246:LEU:HD22	2.01	0.41
1:B:328:LEU:O	1:B:330:VAL:N	2.52	0.41
1:E:239:PRO:HB3	1:E:241:HIS:NE2	2.35	0.41
1:E:298:VAL:HG21	1:E:327:ARG:HD2	2.01	0.41
1:F:264:LYS:HD2	1:F:264:LYS:HA	1.90	0.41
1:H:185:PRO:CB	1:H:210:ARG:HG3	2.49	0.41
1:A:43:HIS:HE1	1:A:263:LYS:H	1.69	0.41
1:C:371:VAL:HG22	1:C:380:LEU:HD22	2.02	0.41
1:D:319:ASP:O	1:D:323:LYS:CB	2.67	0.41
1:E:107:THR:HG23	1:E:110:GLU:H	1.84	0.41
1:A:284:VAL:HG12	1:A:289:MET:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLN:N	1:A:348:LEU:HD23	2.35	0.41
1:A:400:HIS:O	1:A:403:PRO:HG3	2.21	0.41
1:C:270:PHE:O	1:C:274:ILE:HG13	2.21	0.41
1:C:309:ILE:O	1:C:333:ILE:HD12	2.20	0.41
1:D:43:HIS:HE1	1:D:263:LYS:N	2.10	0.41
1:E:353:ARG:HB3	1:E:354:GLU:CA	2.48	0.41
1:G:150:ASP:N	1:G:150:ASP:OD1	2.51	0.41
1:G:397:LYS:HE3	1:G:397:LYS:HB2	1.79	0.41
1:B:314:SER:OG	1:B:338:GLY:HA2	2.21	0.41
1:D:18:PRO:HA	1:D:210:ARG:HH22	1.84	0.41
1:D:274:ILE:HG23	1:D:279:ILE:HB	2.03	0.41
1:D:391:LYS:HB2	1:D:391:LYS:HE3	1.92	0.41
1:D:400:HIS:O	1:D:401:ASN:C	2.58	0.41
1:D:89:LEU:CD2	1:D:246:LEU:HD11	2.50	0.41
1:E:275:GLN:HG2	1:E:301:TYR:CD1	2.32	0.41
1:F:311:CYS:SG	1:F:312:GLY:N	2.93	0.41
1:F:155:ILE:HA	1:G:171:HIS:CD2	2.55	0.41
1:C:103:ASN:HB3	1:C:106:TYR:CE1	2.54	0.41
1:D:116:ASN:O	1:D:119:LYS:NZ	2.50	0.41
1:D:448:ALA:HA	1:D:449:PRO:HD3	1.79	0.41
1:E:288:ILE:HG21	1:E:288:ILE:HD13	1.75	0.41
1:E:369:VAL:HG12	1:E:390:PHE:CE1	2.55	0.41
1:H:145:LYS:HG3	1:H:146:VAL:N	2.36	0.41
1:A:55:GLU:OE2	1:A:59:ARG:NH1	2.54	0.41
1:C:328:LEU:O	1:C:330:VAL:HG13	2.20	0.41
1:D:197:GLY:O	1:D:199:THR:N	2.53	0.41
1:D:266:GLU:OE2	1:D:288:ILE:HG23	2.21	0.41
1:D:439:LEU:HD23	1:D:440:ILE:N	2.36	0.41
1:E:17:PHE:HB3	1:E:24:GLN:OE1	2.21	0.41
1:E:347:ILE:O	1:E:348:LEU:HD23	2.20	0.41
1:F:17:PHE:HA	1:F:18:PRO:HD3	1.94	0.41
1:G:320:ILE:HA	1:G:323:LYS:HG3	2.03	0.41
1:C:215:ARG:HH11	1:C:248:THR:CG2	2.29	0.41
1:C:340:THR:HG22	1:C:341:GLU:H	1.86	0.41
1:C:89:LEU:CD2	1:C:246:LEU:HD11	2.51	0.41
1:D:272:LYS:HB3	1:D:272:LYS:HE2	1.96	0.41
1:D:400:HIS:O	1:D:403:PRO:HD3	2.21	0.41
1:H:37:ASP:HB2	1:H:258:LYS:HE2	2.03	0.41
1:H:282:ILE:HG13	1:H:306:LEU:HD11	2.02	0.41
1:B:239:PRO:HB3	1:B:241:HIS:NE2	2.35	0.41
1:E:294:LYS:HA	1:E:294:LYS:HD2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:LEU:HD12	1:F:260:VAL:O	2.21	0.41
1:G:190:ALA:HB2	1:G:209:HIS:CD2	2.55	0.41
1:G:284:VAL:HB	1:G:288:ILE:HB	2.03	0.41
1:H:333:ILE:HG13	1:H:333:ILE:O	2.21	0.41
1:H:342:THR:CG2	1:H:396:MET:H	2.34	0.41
1:H:203:LYS:HD2	1:H:399:TYR:CD1	2.56	0.41
1:C:403:PRO:O	1:C:407:ARG:HG2	2.21	0.41
1:E:288:ILE:O	1:E:291:TYR:HD1	2.03	0.41
1:E:320:ILE:CD1	1:E:323:LYS:HD2	2.51	0.41
1:F:343:CYS:O	1:F:345:ALA:N	2.50	0.41
1:G:107:THR:HG23	1:G:110:GLU:H	1.85	0.41
1:G:330:VAL:C	1:G:332:GLY:H	2.23	0.41
1:B:284:VAL:HG23	1:B:289:MET:CE	2.51	0.40
1:D:285:PRO:HD2	1:D:288:ILE:HD12	2.03	0.40
1:F:291:TYR:HD1	1:F:291:TYR:HA	1.63	0.40
1:H:149:ILE:HA	1:H:161:VAL:HG23	2.04	0.40
1:H:191:LEU:HD12	1:H:212:ILE:HD11	2.03	0.40
1:B:194:THR:HA	1:B:204:GLY:HA2	2.03	0.40
1:C:230:PRO:HG3	1:C:255:VAL:O	2.21	0.40
1:E:307:THR:HG22	1:E:308:GLU:HG3	2.04	0.40
1:F:13:ARG:HD2	1:F:222:PRO:HD2	2.03	0.40
1:F:292:LEU:HA	1:F:292:LEU:HD12	1.91	0.40
1:H:143:LEU:HA	1:H:143:LEU:HD12	1.68	0.40
1:H:330:VAL:HG12	1:H:332:GLY:H	1.85	0.40
1:A:89:LEU:CD2	1:A:246:LEU:HD11	2.51	0.40
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.84	0.40
1:C:205:VAL:HG11	1:C:342:THR:CG2	2.51	0.40
1:E:270:PHE:CD1	1:E:270:PHE:C	2.95	0.40
1:E:291:TYR:CG	1:E:292:LEU:N	2.89	0.40
1:H:316:LEU:HD23	1:H:316:LEU:HA	1.92	0.40
1:A:135:LYS:O	1:A:138:LYS:HB2	2.21	0.40
1:D:292:LEU:HD22	1:D:328:LEU:HD11	2.03	0.40
1:F:224:TYR:OH	1:F:362:THR:HG23	2.20	0.40
1:G:7:VAL:HG21	1:G:369:VAL:HB	2.02	0.40
1:A:266:GLU:OE1	1:A:288:ILE:HG23	2.22	0.40
1:A:337:TYR:HB2	1:A:347:ILE:CG2	2.52	0.40
1:A:391:LYS:CD	1:A:415:TRP:HD1	2.34	0.40
1:B:41:ASP:CG	1:B:44:THR:HG22	2.42	0.40
1:C:221:ASP:HA	1:C:222:PRO:HD3	1.93	0.40
1:D:337:TYR:HE2	1:D:388:ILE:HD11	1.85	0.40
1:E:365:PRO:O	1:E:366:TYR:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:HIS:CE1	1:F:194:THR:HG1	2.38	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	371/546 (68%)	329 (89%)	29 (8%)	13 (4%)	3	17
1	B	401/546 (73%)	352 (88%)	28 (7%)	21 (5%)	2	10
1	C	405/546 (74%)	359 (89%)	27 (7%)	19 (5%)	2	12
1	D	438/546 (80%)	374 (85%)	44 (10%)	20 (5%)	2	12
1	E	394/546 (72%)	349 (89%)	31 (8%)	14 (4%)	3	16
1	F	413/546 (76%)	362 (88%)	36 (9%)	15 (4%)	3	16
1	G	395/546 (72%)	339 (86%)	35 (9%)	21 (5%)	2	10
1	H	396/546 (72%)	345 (87%)	36 (9%)	15 (4%)	3	15
All	All	3213/4368 (74%)	2809 (87%)	266 (8%)	138 (4%)	2	13

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	GLU
1	A	335	GLN
1	A	401	ASN
1	A	403	PRO
1	B	316	LEU
1	B	337	TYR
1	B	343	CYS
1	B	350	PRO
1	B	386	GLY

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Mol	Chain	Res	Type
1	B	401	ASN
1	C	194	THR
1	C	196	SER
1	C	314	SER
1	C	315	PRO
1	C	329	LYS
1	C	349	SER
1	C	357	LYS
1	C	383	ARG
1	D	198	THR
1	D	227	ARG
1	D	352	ASP
1	D	401	ASN
1	D	446	GLN
1	E	198	THR
1	E	332	GLY
1	E	351	ASN
1	E	352	ASP
1	E	355	LEU
1	F	316	LEU
1	F	318	ARG
1	F	327	ARG
1	F	340	THR
1	F	350	PRO
1	F	354	GLU
1	F	382	PRO
1	F	401	ASN
1	G	198	THR
1	G	265	PHE
1	G	301	TYR
1	G	327	ARG
1	G	375	ASN
1	G	401	ASN
1	H	331	HIS
1	H	400	HIS
1	A	316	LEU
1	B	33	SER
1	B	304	SER
1	B	327	ARG
1	B	347	ILE
1	C	195	SER
1	C	323	LYS

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Mol	Chain	Res	Type
1	C	327	ARG
1	C	351	ASN
1	C	359	ALA
1	D	322	ASP
1	D	332	GLY
1	D	381	GLY
1	D	414	GLY
1	D	432	VAL
1	D	438	GLU
1	E	33	SER
1	E	314	SER
1	F	329	LYS
1	F	332	GLY
1	G	270	PHE
1	G	377	GLY
1	H	33	SER
1	H	265	PHE
1	H	304	SER
1	H	317	GLY
1	H	339	LEU
1	H	425	ASP
1	A	197	GLY
1	A	314	SER
1	B	271	LEU
1	B	329	LYS
1	B	400	HIS
1	D	33	SER
1	D	304	SER
1	D	350	PRO
1	F	33	SER
1	F	198	THR
1	F	331	HIS
1	F	353	ARG
1	G	33	SER
1	G	266	GLU
1	G	331	HIS
1	G	418	THR
1	H	318	ARG
1	H	329	LYS
1	H	341	GLU
1	H	422	GLY
1	A	294	LYS

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Mol	Chain	Res	Type
1	A	364	MET
1	B	313	GLY
1	B	378	LYS
1	C	33	SER
1	C	360	ILE
1	D	403	PRO
1	D	426	GLU
1	E	356	LYS
1	G	400	HIS
1	H	267	GLY
1	H	356	LYS
1	H	426	GLU
1	A	295	SER
1	A	343	CYS
1	B	314	SER
1	B	344	SER
1	B	373	ASP
1	B	383	ARG
1	C	7	VAL
1	C	200	GLY
1	C	319	ASP
1	D	266	GLU
1	D	402	ASN
1	D	430	ILE
1	E	118	SER
1	E	328	LEU
1	G	197	GLY
1	G	315	PRO
1	G	316	LEU
1	G	379	ALA
1	A	312	GLY
1	A	313	GLY
1	B	203	LYS
1	D	356	LYS
1	E	349	SER
1	F	400	HIS
1	G	340	THR
1	G	350	PRO
1	E	313	GLY
1	G	419	GLY
1	G	317	GLY
1	E	290	VAL

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Mol	Chain	Res	Type
1	B	312	GLY
1	C	347	ILE
1	E	360	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	328/471 (70%)	313 (95%)	15 (5%)	27	57
1	B	352/471 (75%)	338 (96%)	14 (4%)	31	62
1	C	355/471 (75%)	339 (96%)	16 (4%)	27	58
1	D	384/471 (82%)	365 (95%)	19 (5%)	25	55
1	E	345/471 (73%)	330 (96%)	15 (4%)	29	59
1	F	361/471 (77%)	346 (96%)	15 (4%)	30	60
1	G	348/471 (74%)	328 (94%)	20 (6%)	20	49
1	H	347/471 (74%)	328 (94%)	19 (6%)	21	50
All	All	2820/3768 (75%)	2687 (95%)	133 (5%)	26	56

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	10	ASP
1	A	44	THR
1	A	45	ASN
1	A	107	THR
1	A	115	LEU
1	A	201	LEU
1	A	203	LYS
1	A	215	ARG
1	A	223	ILE
1	A	244	PHE
1	A	307	THR

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Mol	Chain	Res	Type
1	A	322	ASP
1	A	348	LEU
1	A	408	ASP
1	B	23	LEU
1	B	24	GLN
1	B	47	VAL
1	B	165	VAL
1	B	182	GLU
1	B	226	THR
1	B	244	PHE
1	B	265	PHE
1	B	299	ASP
1	B	333	ILE
1	B	340	THR
1	B	347	ILE
1	B	348	LEU
1	B	401	ASN
1	C	23	LEU
1	C	203	LYS
1	C	215	ARG
1	C	223	ILE
1	C	226	THR
1	C	284	VAL
1	C	327	ARG
1	C	337	TYR
1	C	353	ARG
1	C	357	LYS
1	C	360	ILE
1	C	397	LYS
1	C	402	ASN
1	C	410	LEU
1	C	416	LEU
1	C	421	LEU
1	D	5	ASN
1	D	7	VAL
1	D	122	LEU
1	D	141	ASP
1	D	165	VAL
1	D	167	ARG
1	D	194	THR
1	D	217	VAL
1	D	266	GLU

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Mol	Chain	Res	Type
1	D	268	GLU
1	D	292	LEU
1	D	322	ASP
1	D	324	VAL
1	D	383	ARG
1	D	413	ASP
1	D	421	LEU
1	D	438	GLU
1	D	439	LEU
1	D	441	LYS
1	E	7	VAL
1	E	72	ASN
1	E	141	ASP
1	E	226	THR
1	E	270	PHE
1	E	297	LEU
1	E	298	VAL
1	E	301	TYR
1	E	304	SER
1	E	320	ILE
1	E	326	LYS
1	E	329	LYS
1	E	351	ASN
1	E	360	ILE
1	E	413	ASP
1	F	6	ILE
1	F	72	ASN
1	F	141	ASP
1	F	151	SER
1	F	165	VAL
1	F	220	SER
1	F	244	PHE
1	F	276	ASN
1	F	306	LEU
1	F	311	CYS
1	F	339	LEU
1	F	340	THR
1	F	341	GLU
1	F	380	LEU
1	F	424	TYR
1	G	115	LEU
1	G	135	LYS

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Mol	Chain	Res	Type
1	G	201	LEU
1	G	244	PHE
1	G	268	GLU
1	G	269	PHE
1	G	276	ASN
1	G	292	LEU
1	G	326	LYS
1	G	328	LEU
1	G	339	LEU
1	G	347	ILE
1	G	375	ASN
1	G	376	THR
1	G	378	LYS
1	G	380	LEU
1	G	393	GLN
1	G	397	LYS
1	G	410	LEU
1	G	418	THR
1	H	37	ASP
1	H	107	THR
1	H	115	LEU
1	H	165	VAL
1	H	217	VAL
1	H	265	PHE
1	H	266	GLU
1	H	268	GLU
1	H	270	PHE
1	H	284	VAL
1	H	333	ILE
1	H	340	THR
1	H	346	LEU
1	H	347	ILE
1	H	407	ARG
1	H	417	HIS
1	H	421	LEU
1	H	423	TYR
1	H	424	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN

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Mol	Chain	Res	Type
1	A	43	HIS
1	A	404	GLN
1	B	43	HIS
1	B	95	GLN
1	C	331	HIS
1	D	5	ASN
1	D	43	HIS
1	E	27	GLN
1	E	351	ASN
1	F	8	ASN
1	G	335	GLN
1	H	402	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	377/546 (69%)	-0.20	7 (1%) 66 43	49, 71, 150, 244	0
1	B	405/546 (74%)	0.01	20 (4%) 29 13	43, 86, 182, 250	0
1	C	409/546 (74%)	-0.17	12 (2%) 51 26	50, 76, 169, 239	0
1	D	442/546 (80%)	-0.07	19 (4%) 35 16	41, 68, 155, 256	0
1	E	398/546 (72%)	0.01	24 (6%) 21 9	58, 84, 179, 239	0
1	F	417/546 (76%)	-0.14	14 (3%) 45 22	45, 72, 160, 221	0
1	G	401/546 (73%)	-0.13	16 (3%) 38 18	30, 74, 163, 223	0
1	H	400/546 (73%)	-0.07	17 (4%) 35 16	50, 74, 170, 260	0
All	All	3249/4368 (74%)	-0.09	129 (3%) 38 18	30, 77, 170, 260	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	ASN	13.1
1	D	429	PHE	8.2
1	H	317	GLY	6.9
1	D	427	ASP	6.9
1	D	317	GLY	6.5
1	E	316	LEU	6.0
1	E	314	SER	5.4
1	D	428	ARG	5.4
1	B	351	ASN	5.1
1	B	314	SER	5.1
1	B	338	GLY	5.0
1	H	361	GLY	5.0
1	D	351	ASN	4.9
1	H	413	ASP	4.8
1	C	361	GLY	4.8
1	F	316	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	196	SER	4.8
1	E	354	GLU	4.8
1	E	357	LYS	4.5
1	C	318	ARG	4.5
1	D	318	ARG	4.4
1	A	401	ASN	4.4
1	C	319	ASP	4.4
1	F	423	TYR	4.3
1	E	337	TYR	4.2
1	B	376	THR	4.2
1	C	337	TYR	4.1
1	C	421	LEU	4.0
1	E	313	GLY	4.0
1	F	421	LEU	3.9
1	D	384	GLU	3.9
1	B	370	LYS	3.9
1	B	198	THR	3.8
1	B	203	LYS	3.8
1	F	317	GLY	3.7
1	E	356	LYS	3.7
1	E	358	GLY	3.6
1	G	304	SER	3.6
1	H	337	TYR	3.5
1	E	415	TRP	3.4
1	B	412	LYS	3.4
1	F	298	VAL	3.4
1	E	293	ALA	3.4
1	A	317	GLY	3.4
1	H	360	ILE	3.3
1	B	375	ASN	3.3
1	G	380	LEU	3.3
1	C	360	ILE	3.3
1	E	419	GLY	3.3
1	B	389	CYS	3.2
1	B	322	ASP	3.2
1	B	313	GLY	3.2
1	E	338	GLY	3.1
1	D	297	LEU	3.1
1	E	421	LEU	3.1
1	D	435	ARG	3.1
1	H	420	ASP	3.1
1	E	294	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	199	THR	3.0
1	A	318	ARG	3.0
1	C	317	GLY	3.0
1	C	385	LYS	3.0
1	E	317	GLY	2.9
1	F	291	TYR	2.8
1	G	295	SER	2.8
1	G	318	ARG	2.7
1	D	426	GLU	2.7
1	D	296	PRO	2.7
1	E	420	ASP	2.7
1	E	198	THR	2.6
1	B	377	GLY	2.6
1	B	296	PRO	2.6
1	D	445	TYR	2.6
1	D	298	VAL	2.6
1	G	7	VAL	2.6
1	H	399	TYR	2.6
1	F	360	ILE	2.6
1	F	296	PRO	2.6
1	D	300	GLU	2.5
1	B	373	ASP	2.5
1	G	420	ASP	2.5
1	A	296	PRO	2.5
1	A	370	LYS	2.5
1	G	8	ASN	2.5
1	E	407	ARG	2.5
1	G	200	GLY	2.5
1	H	339	LEU	2.5
1	E	199	THR	2.4
1	G	332	GLY	2.4
1	F	312	GLY	2.4
1	D	302	ASN	2.4
1	H	314	SER	2.3
1	C	312	GLY	2.3
1	H	353	ARG	2.3
1	G	377	GLY	2.3
1	E	408	ASP	2.3
1	H	199	THR	2.3
1	G	350	PRO	2.3
1	B	421	LEU	2.3
1	E	411	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	299	ASP	2.2
1	F	313	GLY	2.2
1	H	358	GLY	2.2
1	D	385	LYS	2.2
1	H	292	LEU	2.2
1	B	297	LEU	2.2
1	C	292	LEU	2.2
1	D	446	GLN	2.2
1	E	418	THR	2.2
1	B	408	ASP	2.2
1	C	351	ASN	2.2
1	H	415	TRP	2.2
1	B	270	PHE	2.1
1	C	293	ALA	2.1
1	F	314	SER	2.1
1	G	305	SER	2.1
1	H	422	GLY	2.1
1	H	269	PHE	2.1
1	F	356	LYS	2.1
1	A	203	LYS	2.1
1	D	199	THR	2.1
1	E	355	LEU	2.1
1	G	317	GLY	2.1
1	H	196	SER	2.1
1	G	376	THR	2.1
1	F	372	ILE	2.1
1	B	387	GLU	2.0
1	F	354	GLU	2.0
1	D	437	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.