



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:56 AM UTC

PDB ID : 6ABH / pdb_00006abh
Title : Structure of a natural red emitting luciferase from Phrixothrix hirtus (P1 crystal form)
Authors : Carrasco-Lopez, C.; Panjikar, 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

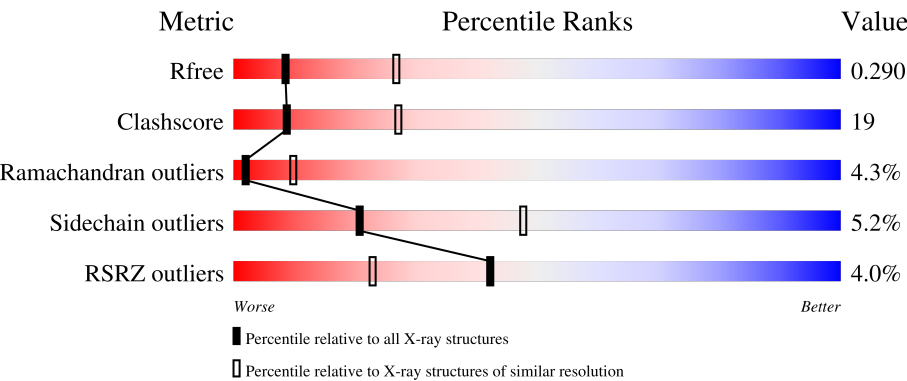
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	546	2% 44% 21% •• 31%
1	B	546	4% 47% 23% •• 26%
1	C	546	3% 45% 26% • 25%
1	D	546	4% 47% 28% 5% • 19%
1	E	546	2% 41% 28% •• 27%

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Mol	Chain	Length	Quality of chain
1	F	546	 3% 49% 24% 24%
1	G	546	 3% 46% 23% 27%
1	H	546	 3% 41% 27% 27%

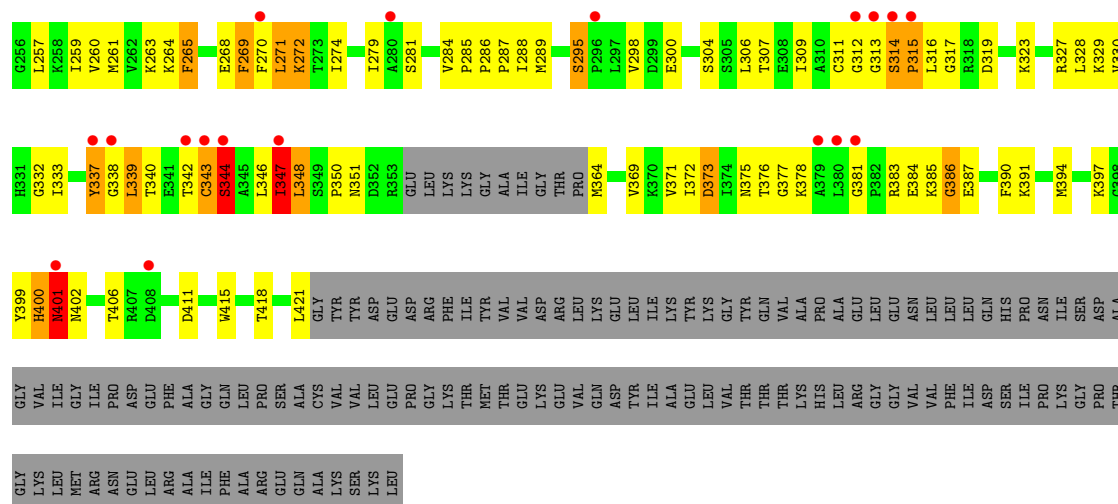
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25451 atoms, of which 0 are hydrogens and 0 are deuteriums.

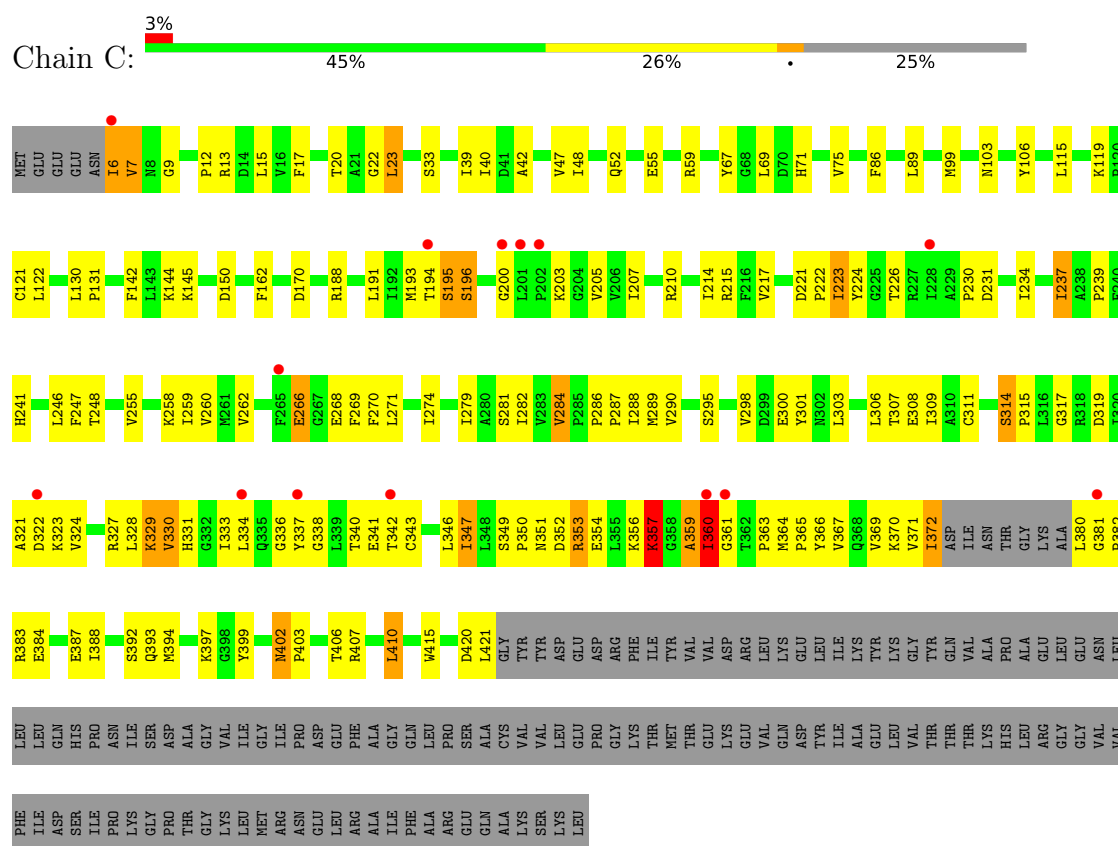
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

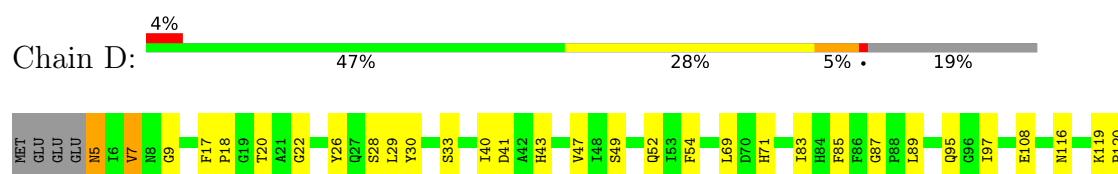
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2955	1915	487	535	18			
1	B	405	Total	C	N	O	S	0	0	0
			3170	2047	527	577	19			
1	C	409	Total	C	N	O	S	0	0	0
			3199	2069	531	580	19			
1	D	442	Total	C	N	O	S	0	0	0
			3480	2251	576	634	19			
1	E	398	Total	C	N	O	S	0	0	0
			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			

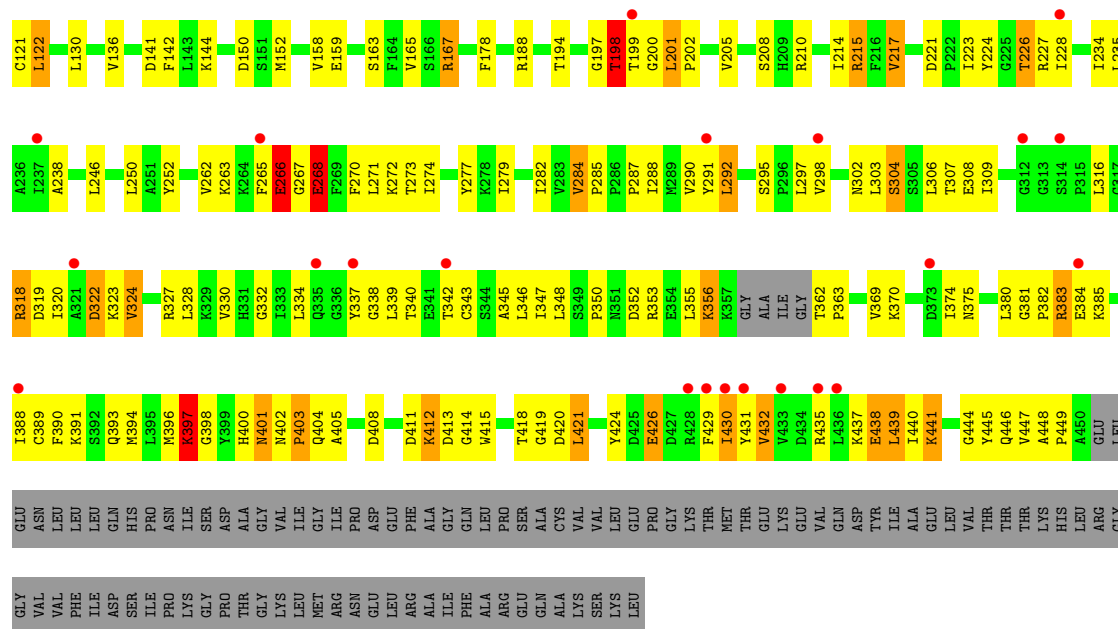


• Molecule 1: Red-bioluminescence eliciting luciferase

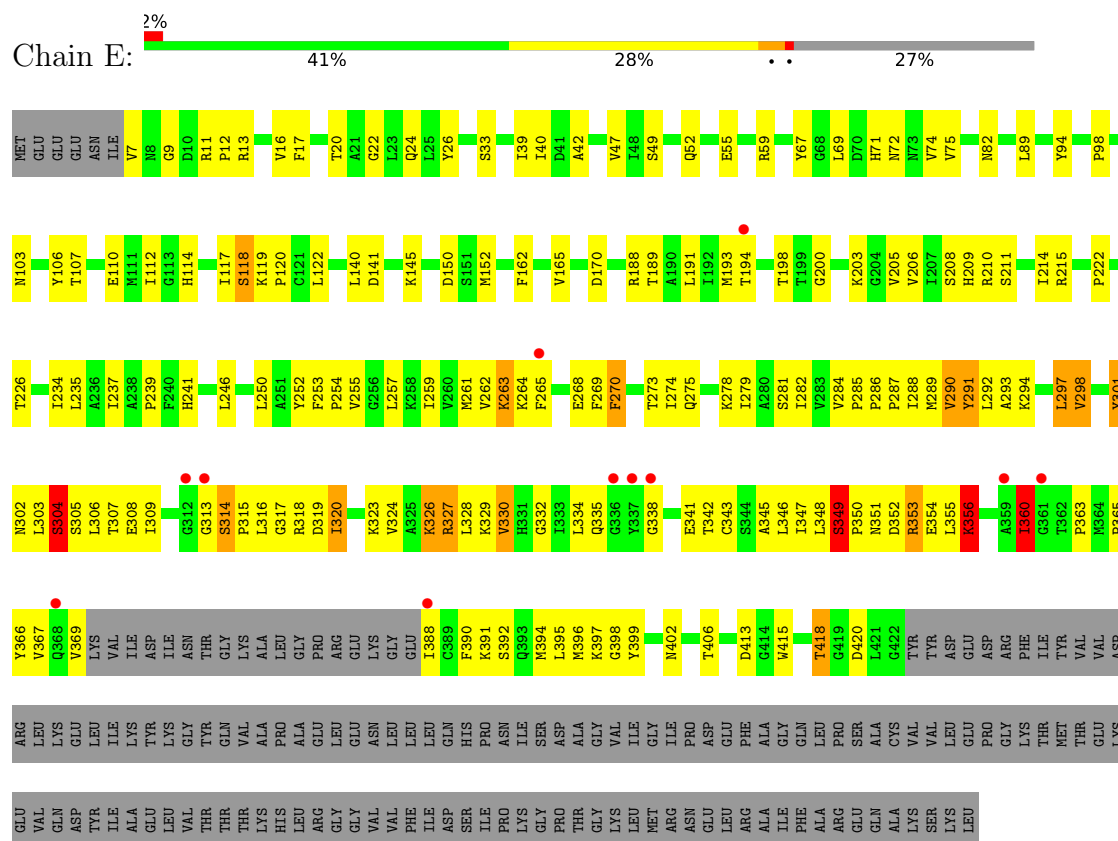


• Molecule 1: Red-bioluminescence eliciting luciferase



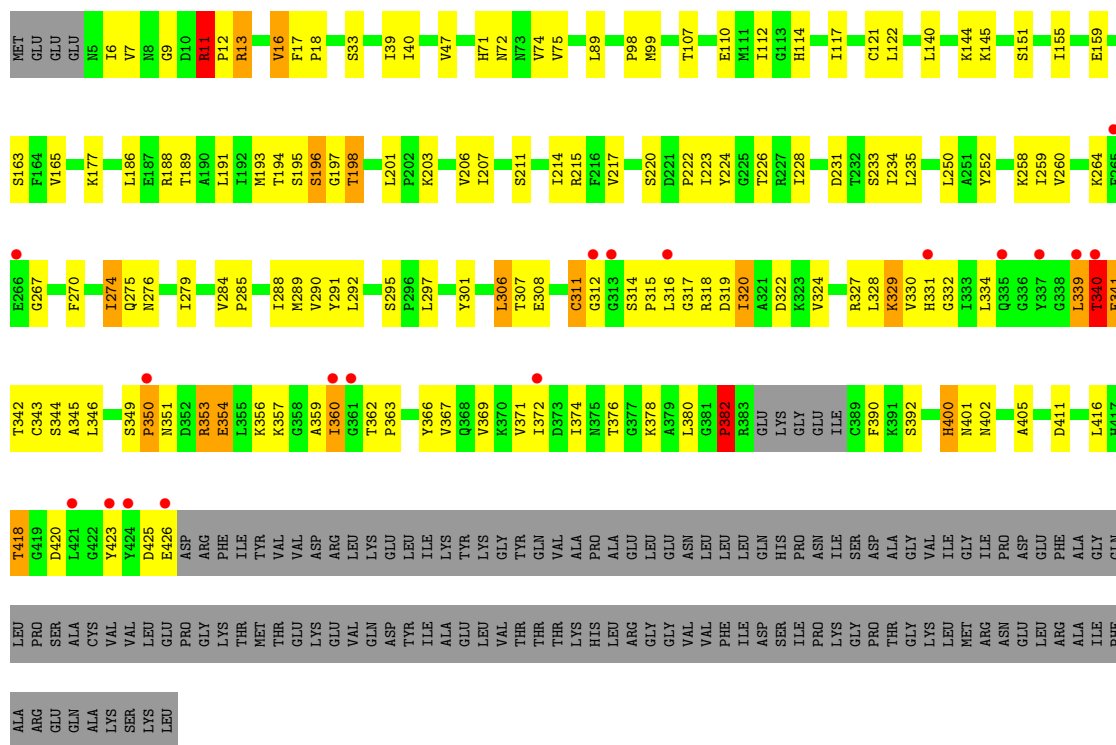


• Molecule 1: Red-bioluminescence eliciting luciferase

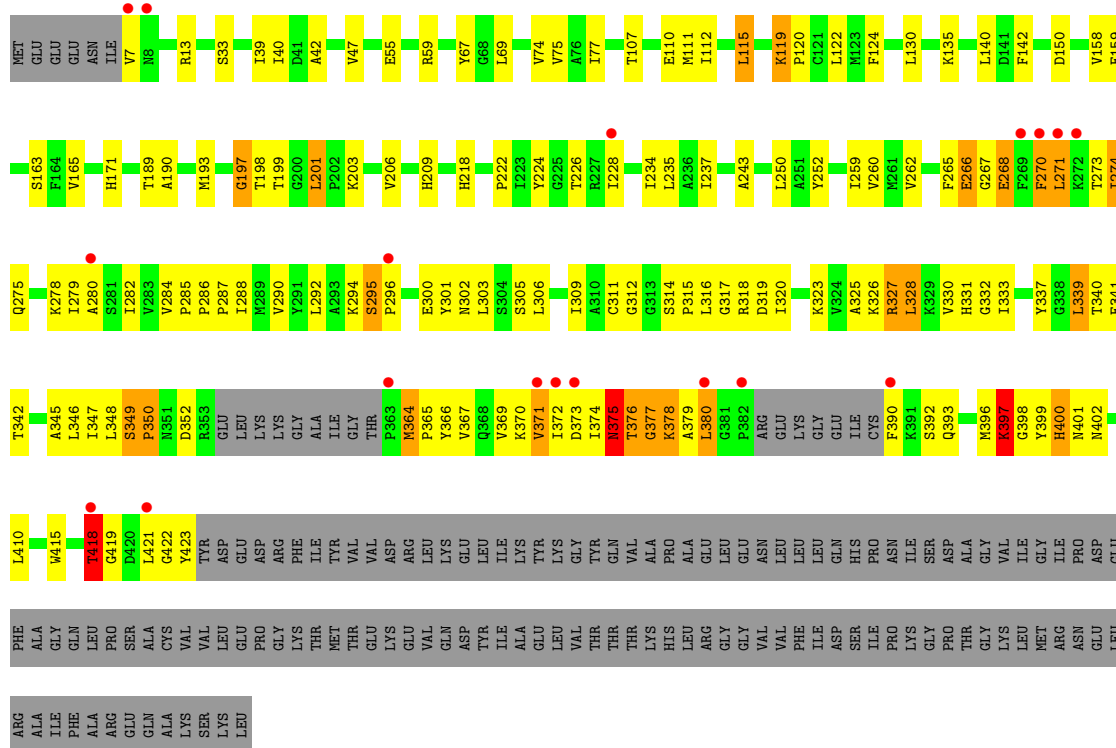


• Molecule 1: Red-bioluminescence eliciting luciferase





• Molecule 1: Red-bioluminescence eliciting luciferase



• Molecule 1: Red-bioluminescence eliciting luciferase



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 0.260 , 0.290	Depositor DCC
R_{free} test set	955 reflections (0.96%)	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)	0.31 , 67.6	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	0.77	0/3026	1.13	16/4100 (0.4%)
1	B	0.73	0/3245	1.07	17/4398 (0.4%)
1	C	0.75	0/3275	1.10	7/4438 (0.2%)
1	D	0.81	1/3563 (0.0%)	1.13	17/4829 (0.4%)
1	E	0.69	0/3185	1.08	13/4318 (0.3%)
1	F	0.75	1/3340 (0.0%)	1.17	21/4528 (0.5%)
1	G	0.72	0/3213	1.08	13/4356 (0.3%)
1	H	0.76	0/3215	1.17	17/4359 (0.4%)
All	All	0.75	2/26062 (0.0%)	1.12	121/35326 (0.3%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	120	PRO	C-O	-5.83	1.17	1.23
1	F	196	SER	CA-C	5.83	1.55	1.52

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	341	GLU	N-CA-C	-15.38	78.05	110.80
1	H	349	SER	CA-C-N	12.75	132.73	119.85
1	H	349	SER	C-N-CA	12.75	132.73	119.85
1	H	398	GLY	N-CA-C	-12.23	98.88	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	305	SER	N-CA-C	-10.14	100.65	113.23
1	E	349	SER	CA-C-N	-9.80	109.95	119.76
1	E	349	SER	C-N-CA	-9.80	109.95	119.76
1	F	349	SER	CA-C-N	9.62	131.87	119.84
1	F	349	SER	C-N-CA	9.62	131.87	119.84
1	C	266	GLU	N-CA-C	9.44	121.26	110.97
1	C	86	PHE	N-CA-C	-8.80	97.50	110.52
1	D	404	GLN	N-CA-C	-8.33	102.56	112.89
1	F	267	GLY	N-CA-C	8.17	121.16	111.35
1	H	201	LEU	CA-C-N	-7.94	112.17	120.03
1	H	201	LEU	C-N-CA	-7.94	112.17	120.03
1	F	11	ARG	CA-C-N	7.72	127.71	119.76
1	F	11	ARG	C-N-CA	7.72	127.71	119.76
1	F	314	SER	CA-C-N	7.46	129.17	119.84
1	F	314	SER	C-N-CA	7.46	129.17	119.84
1	E	353	ARG	N-CA-C	-7.42	98.44	108.24
1	A	364	MET	CA-C-N	7.40	127.39	119.76
1	A	364	MET	C-N-CA	7.40	127.39	119.76
1	G	349	SER	CA-C-N	7.24	128.89	119.84
1	G	349	SER	C-N-CA	7.24	128.89	119.84
1	E	304	SER	N-CA-C	-7.19	101.47	111.39
1	B	381	GLY	CA-C-N	7.03	128.63	119.84
1	B	381	GLY	C-N-CA	7.03	128.63	119.84
1	H	406	THR	N-CA-C	-6.96	103.69	111.28
1	D	201	LEU	CA-C-N	-6.96	112.83	119.85
1	D	201	LEU	C-N-CA	-6.96	112.83	119.85
1	A	405	ALA	N-CA-C	-6.83	104.42	112.89
1	C	314	SER	CA-C-N	6.76	128.29	119.84
1	C	314	SER	C-N-CA	6.76	128.29	119.84
1	E	11	ARG	CA-C-N	6.70	127.10	119.93
1	E	11	ARG	C-N-CA	6.70	127.10	119.93
1	G	271	LEU	N-CA-C	-6.67	104.09	111.36
1	D	120	PRO	CB-CA-C	-6.55	102.50	111.21
1	B	344	SER	N-CA-C	6.42	124.47	110.80
1	E	269	PHE	N-CA-C	-6.36	104.39	111.71
1	G	303	LEU	N-CA-C	-6.35	105.29	113.16
1	G	295	SER	CA-C-N	-6.34	111.92	119.84
1	G	295	SER	C-N-CA	-6.34	111.92	119.84
1	D	412	LYS	N-CA-C	-6.33	101.12	110.48
1	D	226	THR	N-CA-C	6.21	120.85	113.28
1	C	388	ILE	N-CA-C	6.16	117.46	108.53
1	D	303	LEU	N-CA-C	-6.11	105.69	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	LYS	N-CA-C	-6.11	103.94	111.33
1	F	12	PRO	CA-C-O	-6.10	114.38	121.34
1	D	268	GLU	N-CA-C	-6.03	105.93	113.28
1	B	119	LYS	CA-C-N	6.01	125.77	119.76
1	B	119	LYS	C-N-CA	6.01	125.77	119.76
1	G	119	LYS	CA-C-N	6.01	126.48	119.99
1	G	119	LYS	C-N-CA	6.01	126.48	119.99
1	F	201	LEU	N-CA-C	-5.99	102.55	110.40
1	H	336	GLY	CA-C-N	5.97	131.84	122.17
1	H	336	GLY	C-N-CA	5.97	131.84	122.17
1	H	262	VAL	N-CA-C	5.94	117.04	108.48
1	B	397	LYS	N-CA-C	-5.93	105.80	113.16
1	F	117	ILE	N-CA-C	5.91	116.08	110.53
1	B	269	PHE	N-CA-C	-5.88	104.86	111.28
1	H	358	GLY	N-CA-C	-5.88	105.36	112.48
1	H	348	LEU	N-CA-C	5.87	118.80	109.65
1	A	295	SER	CA-C-N	5.84	125.46	119.56
1	A	295	SER	C-N-CA	5.84	125.46	119.56
1	D	375	ASN	N-CA-C	5.82	119.69	112.59
1	G	273	THR	N-CA-C	5.80	117.61	111.28
1	F	382	PRO	CA-C-N	-5.75	111.35	121.70
1	F	382	PRO	C-N-CA	-5.75	111.35	121.70
1	D	87	GLY	CA-C-N	5.71	125.39	119.05
1	D	87	GLY	C-N-CA	5.71	125.39	119.05
1	A	12	PRO	N-CA-C	5.70	122.24	113.75
1	F	411	ASP	N-CA-C	-5.69	102.87	110.55
1	F	13	ARG	N-CA-C	-5.67	106.52	113.50
1	H	295	SER	CA-C-N	5.61	124.96	118.85
1	H	295	SER	C-N-CA	5.61	124.96	118.85
1	F	341	GLU	N-CA-CB	5.58	119.92	110.49
1	D	238	ALA	CA-C-N	5.52	125.84	119.93
1	D	238	ALA	C-N-CA	5.52	125.84	119.93
1	A	184	ASP	CA-C-N	5.52	125.61	119.87
1	A	184	ASP	C-N-CA	5.52	125.61	119.87
1	F	418	THR	N-CA-C	5.51	120.46	111.37
1	C	420	ASP	N-CA-C	5.51	117.88	109.95
1	D	353	ARG	N-CA-C	-5.49	106.56	113.20
1	A	266	GLU	CA-C-N	5.47	126.45	121.31
1	A	266	GLU	C-N-CA	5.47	126.45	121.31
1	B	253	PHE	CA-C-N	-5.47	114.03	119.56
1	B	253	PHE	C-N-CA	-5.47	114.03	119.56
1	F	320	ILE	N-CA-C	-5.47	105.04	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	TYR	CA-CB-CG	-5.44	104.10	113.90
1	F	405	ALA	N-CA-C	-5.43	106.15	112.89
1	A	221	ASP	CA-C-N	5.43	125.52	119.87
1	A	221	ASP	C-N-CA	5.43	125.52	119.87
1	F	314	SER	N-CA-C	5.41	121.76	109.81
1	E	418	THR	N-CA-C	5.40	116.97	111.14
1	H	286	PRO	N-CA-C	5.39	117.27	110.70
1	B	295	SER	N-CA-C	5.38	118.01	109.40
1	B	7	VAL	CA-C-N	-5.35	113.85	122.24
1	B	7	VAL	C-N-CA	-5.35	113.85	122.24
1	E	360	ILE	CA-C-N	-5.34	118.05	122.16
1	E	360	ILE	C-N-CA	-5.34	118.05	122.16
1	A	267	GLY	N-CA-C	5.34	119.19	111.24
1	B	205	VAL	N-CA-C	5.30	116.93	108.87
1	G	364	MET	N-CA-C	5.28	117.66	110.01
1	B	418	THR	N-CA-C	5.27	117.83	111.40
1	E	291	TYR	N-CA-C	-5.27	105.71	111.82
1	D	26	TYR	N-CA-C	-5.26	105.44	111.07
1	G	397	LYS	N-CA-C	-5.23	107.07	112.93
1	F	274	ILE	CB-CA-C	-5.21	105.30	111.97
1	H	333	ILE	N-CA-C	-5.21	100.90	108.97
1	H	418	THR	N-CA-C	5.20	118.09	111.69
1	D	397	LYS	N-CA-C	-5.20	106.72	113.16
1	E	12	PRO	CA-C-O	-5.18	115.67	121.32
1	A	328	LEU	N-CA-C	-5.15	103.60	110.55
1	G	318	ARG	N-CA-C	-5.10	106.90	112.72
1	D	28	SER	N-CA-C	5.08	116.81	111.28
1	A	400	HIS	N-CA-C	5.06	117.38	110.55
1	C	352	ASP	N-CA-C	-5.05	107.61	112.97
1	B	315	PRO	CA-C-N	5.05	131.18	121.54
1	B	315	PRO	C-N-CA	5.05	131.18	121.54
1	H	350	PRO	N-CA-C	5.03	119.37	111.38
1	G	274	ILE	CB-CA-C	-5.01	105.56	111.97

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	111	0
1	B	3170	0	3205	100	0
1	C	3199	0	3246	120	0
1	D	3480	0	3513	144	0
1	E	3110	0	3143	135	0
1	F	3262	0	3293	105	0
1	G	3137	0	3167	108	0
1	H	3138	0	3150	145	0
All	All	25451	0	25707	956	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (956) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:205:VAL:HG13	1:D:396:MET:HE3	1.53	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:HD2	1:D:215:ARG:O	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:286:PRO:HG3	1:H:314:SER:HB3	1.61	0.82
1:H:289:MET:HG2	1:H:316:LEU:HD11	1.60	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD1	1:H:423:TYR:H	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:356:LYS:O	1:C:359:ALA:CB	2.43	0.66
1:D:435:ARG:HB2	1:D:437:LYS:HZ2	1.60	0.66
1:F:340:THR:HG1	1:F:344:SER:HA	1.56	0.66
1:F:425:ASP:C	1:F:426:GLU:HG2	2.20	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:HH11	1:C:353:ARG:CB	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:SER:OG	1:C:196:SER:N	2.27	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:HH11	1:C:353:ARG:HG2	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:C:289:MET:HE2	1:C:311:CYS:HB2	1.78	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:C:356:LYS:O	1:C:357:LYS:C	2.41	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:H:218:HIS:CG	1:H:364:MET:HE3	2.33	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
1:A:59:ARG:NH2	1:A:170:ASP:O	2.32	0.63
1:A:289:MET:HE2	1:A:311:CYS:HB2	1.81	0.63
1:E:193:MET:HE1	1:E:246:LEU:HD22	1.81	0.63
1:G:75:VAL:HG12	1:G:122:LEU:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:382:PRO:C	1:C:384:GLU:H	2.09	0.61
1:D:297:LEU:HD12	1:D:297:LEU:C	2.26	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: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:A:403:PRO:C	1:A:405:ALA:H	2.10	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:D:295:SER:HG	1:D:297:LEU:HG	1.67	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:HD22	1:F:416:LEU:CD2	2.30	0.59
1:F:339:LEU:HD13	1:F:416:LEU:HD21	1.83	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: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: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:B:284:VAL:HG23	1:B:289:MET:HE1	1.84	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:G:295:SER:O	1:G:295:SER:OG	2.10	0.58
1:H:215:ARG:HH21	1:H:248:THR:HA	1.68	0.58
1:H:215:ARG:HB2	1:H:394:MET:HE3	1.84	0.58
1:B:342:THR:O	1:B:343:CYS:HB2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:TYR:HE1	1:B:348:LEU:O	1.86	0.58
1:B:289:MET:HE3	1:B:311:CYS:HB3	1.84	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
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:H:289:MET:HE3	1:H:324:VAL:HG21	1.86	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:40:ILE:HG12	1:H:47:VAL:HG22	1.87	0.57
1:H:265:PHE:N	1:H:265:PHE:CD1	2.73	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:G:218:HIS:CG	1:G:364:MET:HE3	2.40	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: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:B:286:PRO:HG2	1:B:287:PRO:HD3	1.88	0.56
1:E:292:LEU:HG	1:E:327:ARG:HH11	1.69	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:C:356:LYS:C	1:C:357:LYS:O	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:370:LYS:HZ3	1:D:415:TRP:CD1	2.23	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: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:G:197:GLY:C	1:G:199:THR:H	2.14	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:B:387:GLU:H	1:B:387:GLU:CD	2.15	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:N	1:D:5:ASN:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:32:TYR:C	1:A:34:TYR:H	2.16	0.53
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:H:330:VAL:C	1:H:332:GLY:H	2.16	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:206:VAL:HG12	1:E:398:GLY:O	2.08	0.53
1:E:292:LEU:HD22	1:E:323:LYS:HB3	1.90	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:H:334:LEU:C	1:H:349:SER:HB2	2.33	0.53
1:B:191:LEU:HD22	1:B:193:MET:HE2	1.90	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:9:GLY:HA2	1:D:363:PRO:HB2	1.91	0.53
1:D:403:PRO:HB2	1:D:405:ALA:H	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:37:ASP:HA	1:H:47:VAL:HG11	1.90	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: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:E:343:CYS:SG	1:E:394:MET:HE3	2.50	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:107:THR:HG23	1:A:110:GLU:CD	2.35	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:6:ILE:HG12	1:C:380:LEU:O	2.10	0.51
1:C:347:ILE:CG2	1:C:361:GLY:CA	2.89	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:A:345:ALA:C	1:A:346:LEU:HD12	2.35	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:340:THR:C	1:H:342:THR:H	2.18	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:67:TYR:HD2	1:C:69:LEU:HD13	1.75	0.50
1:C:308:GLU:HG2	1:C:331:HIS:HE1	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:210:ARG:HH22	1:H:393:GLN:CD	2.20	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
1:E:327:ARG:C	1:E:329:LYS:H	2.20	0.49
1:F:307:THR:HG22	1:F:308:GLU:HG3	1.94	0.49
1:H:107:THR:HG1	1:H:109:ARG:HG3	1.78	0.49
1:D:306:LEU:HG	1:D:309:ILE:HD11	1.94	0.49
1:G:372:ILE:O	1:G:373:ASP:C	2.56	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:G:345:ALA:C	1:G:346:LEU:HD12	2.37	0.49
1:F:346:LEU:HD12	1:F:390:PHE:CD2	2.48	0.49
1:G:193:MET:HE1	1:G:243:ALA:HA	1.95	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: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: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: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:B:152:MET:HE1	1:B:162:PHE:CD1	2.47	0.48
1:C:71:HIS:HB3	1:C:188:ARG:NH1	2.28	0.48
1:E:302:ASN:C	1:E:303:LEU:HD12	2.38	0.48
1:B:285:PRO:HD2	1:B:288:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:401:ASN:C	1:A:403:PRO:HD3	2.39	0.48
1:B:369:VAL:HG12	1:B:390:PHE:HE1	1.78	0.48
1:C:6:ILE:HG23	1:C:381:GLY:HA2	1.96	0.48
1:C:308:GLU:HG2	1:C:331:HIS:CE1	2.48	0.48
1:B:83:ILE:HD13	1:B:261:MET:CE	2.43	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:C:370:LYS:HZ1	1:C:415:TRP:CD1	2.32	0.48
1:A:59:ARG:NH2	1:A:173:PHE:HB3	2.29	0.47
1:E:289:MET:C	1:E:291:TYR:H	2.21	0.47
1:F:89:LEU:HD11	1:F:191:LEU:HD21	1.95	0.47
1:F:234:ILE:HD13	1:F:252:TYR:CE1	2.48	0.47
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:13:ARG:HD2	1:G:222:PRO:HD2	1.95	0.47
1:G:197:GLY:O	1:G:199:THR:N	2.47	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:B:295:SER:OG	1:B:298:VAL:HB	2.14	0.47
1:B:386:GLY:C	1:B:421:LEU:HG	2.39	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:D:215:ARG:HD2	1:D:215:ARG:C	2.35	0.47
1:D:274:ILE:HA	1:D:279:ILE:HD12	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:150:ASP:OD1	1:H:150:ASP:N	2.47	0.47
1:H:303:LEU:HD22	1:H:328:LEU:CD2	2.45	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:E:341:GLU:OE2	1:E:396:MET:HE1	2.15	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:284:VAL:CG2	1:E:289:MET:HE3	2.45	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:E:263:LYS:HE2	1:E:263:LYS:HB2	1.68	0.47
1:F:250:LEU:HA	1:F:250:LEU:HD23	1.47	0.47
1:A:101:THR:OG1	1:A:193:MET:HE3	2.15	0.46
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:H:330:VAL:C	1:H:332:GLY:N	2.73	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
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:N	1:H:341:GLU:OE1	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:C:343:CYS:SG	1:C:394:MET:HE3	2.55	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:29:LEU:HD23	1:D:54:PHE:HA	1.98	0.46
1:D:318:ARG:O	1:D:322:ASP:OD2	2.33	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:B:306:LEU:HD12	1:B:306:LEU:HA	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:GLU:HG3	1:F:329:LYS:HD3	1.98	0.46
1:D:400:HIS:O	1:D:401:ASN:C	2.58	0.46
1:G:330:VAL:C	1:G:332:GLY:H	2.23	0.46
1:D:316:LEU:O	1:D:320:ILE:HD12	2.15	0.46
1:E:152:MET:HE1	1:E:162:PHE:CD2	2.51	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:32:TYR:O	1:A:34:TYR:N	2.47	0.46
1:A:174:ASP:OD2	1:A:177:LYS:NZ	2.47	0.46
1:D:250:LEU:HD23	1:D:250:LEU:HA	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:B:82:ASN:C	1:B:261:MET:HE1	2.41	0.45
1:F:270:PHE:O	1:F:274:ILE:HG13	2.15	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:421:LEU:HD23	1:D:438:GLU:O	2.16	0.45
1:H:198:THR:C	1:H:199:THR:HG1	2.24	0.45
1:H:311:CYS:O	1:H:335:GLN:HB3	2.16	0.45
1:H:325:ALA:CB	1:H:332:GLY:HA2	2.47	0.45
1:H:348:LEU:HD13	1:H:364:MET:HE2	1.97	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:E:270:PHE:CD1	1:E:270:PHE:C	2.95	0.45
1:F:7:VAL:HB	1:F:369:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:201:LEU:HD12	1:G:203:LYS:HZ2	1.81	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:B:41:ASP:CG	1:B:44:THR:HG22	2.42	0.45
1:D:201:LEU:HD12	1:D:202:PRO:HD2	1.98	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: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: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:HD3	1:E:326:LYS:HA	1.61	0.45
1:H:397:LYS:HA	1:H:397:LYS:HD3	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
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:A:171:HIS:CD2	1:H:155:ILE:HA	2.52	0.44
1:B:89:LEU:CD1	1:B:99:MET:HG2	2.47	0.44
1:B:300:GLU:HG2	1:C:329:LYS:NZ	2.33	0.44
1:D:396:MET:HE2	1:D:398:GLY:C	2.43	0.44
1:E:250:LEU:HA	1:E:250:LEU:HD12	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:200:GLY:HA3	1:E:203:LYS:HZ1	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:191:LEU:HD22	1:E:193:MET:HE2	2.00	0.44
1:F:328:LEU:O	1:F:329:LYS:C	2.60	0.44
1:H:270:PHE:CD1	1:H:270:PHE:C	2.95	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:A:408:ASP:OD1	1:A:408:ASP:C	2.61	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:E:345:ALA:C	1:E:346:LEU:HD12	2.43	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
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:H:343:CYS:C	1:H:344:SER:HG	2.22	0.44
1:A:111:MET:HG3	1:A:115:LEU:HD22	2.00	0.43
1:C:382:PRO:C	1:C:384:GLU:N	2.75	0.43
1:E:285:PRO:HB2	1:E:287:PRO:HD2	1.99	0.43
1:F:371:VAL:HG11	1:F:423:TYR:HD1	1.77	0.43
1:H:15:LEU:HD23	1:H:15:LEU:HA	1.81	0.43
1:A:155:ILE:HA	1:H:171:HIS:CD2	2.53	0.43
1:C:89:LEU:HD21	1:C:246:LEU:HD11	2.00	0.43
1:C:207:ILE:HD13	1:C:247:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:339:LEU:HD22	1:D:340:THR:N	2.34	0.43
1:H:328:LEU:O	1:H:329:LYS:C	2.61	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:HA	1:E:264:LYS:HD2	1.86	0.43
1:F:107:THR:CG2	1:F:110:GLU:H	2.32	0.43
1:A:58:CYS:O	1:A:62:VAL:HG23	2.19	0.43
1:A:152:MET:O	1:H:162:PHE:HZ	2.02	0.43
1:A:365:PRO:O	1:A:366:TYR:HB2	2.17	0.43
1:B:122:LEU:HD12	1:B:123:MET:H	1.82	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: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:D:198:THR:C	1:D:200:GLY:H	2.27	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:F:343:CYS:O	1:F:344:SER:OG	2.32	0.43
1:G:339:LEU:O	1:G:342:THR:OG1	2.33	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:62:VAL:HG21	1:A:173:PHE:HE2	1.83	0.43
1:A:391:LYS:HE3	1:A:391:LYS:HB3	1.85	0.43
1:D:210:ARG:HG2	1:D:393:GLN:HB3	2.01	0.43
1:E:82:ASN:C	1:E:261:MET:HE1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:318:ARG:HG3	1:E:318:ARG:O	2.18	0.43
1:B:150:ASP:OD1	1:B:150:ASP:N	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:OE1	1:G:341:GLU:N	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:E:342:THR:HG23	1:E:396:MET:HE2	2.01	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: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:197:GLY:C	1:G:199:THR:N	2.77	0.42
1:G:306:LEU:HD12	1:G:306:LEU:HA	1.69	0.42
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:197:GLY:O	1:F:198:THR:C	2.62	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:B:240:PHE:CE2	1:B:261:MET:HE2	2.53	0.42
1:C:307:THR:HG22	1:C:308:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:CYS:SG	1:D:394:MET:HE3	2.59	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:C:89:LEU:CD1	1:C:99:MET:HG2	2.48	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:B:27:GLN:HG3	1:H:13:ARG:O	2.20	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:H:413:ASP:N	1:H:415:TRP:HD1	2.17	0.42
1:B:375:ASN:OD1	1:B:375:ASN:N	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:HD12	1:E:316:LEU:O	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:HD23	1:C:115:LEU:HA	1.88	0.42
1:C:406:THR:O	1:C:410:LEU:N	2.27	0.42
1:D:30:TYR:CE2	1:F:11:ARG:HG2	2.54	0.42
1:E:270:PHE:CE1	1:E:274:ILE:HD11	2.50	0.42
1:E:306:LEU:HD12	1:E:306:LEU:HA	1.69	0.42
1:E:354:GLU:O	1:E:356:LYS:N	2.53	0.42
1:F:418:THR:OG1	1:F:420:ASP:O	2.38	0.42
1:B:193:MET:HE1	1:B:246:LEU:HD22	2.02	0.42
1:B:224:TYR:HD1	1:B:348:LEU:HD12	1.84	0.42
1:C:150:ASP:OD1	1:C:150:ASP:N	2.48	0.42
1:D:41:ASP:OD2	1:D:263:LYS:NZ	2.47	0.42
1:D:150:ASP:OD1	1:D:150:ASP:N	2.48	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:193:MET:HE1	1:H:246:LEU:HD23	2.02	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:404:GLN:HG3	1:H:405:ALA:N	2.34	0.42
1:A:315:PRO:O	1:A:317:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:396:MET:C	1:H:398:GLY:H	2.28	0.41
1:A:284:VAL:HG12	1:A:289:MET:HG2	2.01	0.41
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:B:289:MET:HE2	1:B:289:MET:HB2	1.60	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:OD1	1:G:150:ASP:N	2.51	0.41
1:G:397:LYS:HB2	1:G:397:LYS:HE3	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:89:LEU:CD2	1:D:246:LEU:HD11	2.50	0.41
1:D:274:ILE:HG23	1:D:279:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:LYS:HE3	1:D:391:LYS:HB2	1.92	0.41
1:E:275:GLN:HG2	1:E:301:TYR:CD1	2.32	0.41
1:F:155:ILE:HA	1:G:171:HIS:CD2	2.55	0.41
1:F:311:CYS:SG	1:F:312:GLY:N	2.93	0.41
1:A:403:PRO:C	1:A:405:ALA:N	2.77	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:302:ASN:C	1:D:304:SER:H	2.25	0.41
1:D:448:ALA:HA	1:D:449:PRO:HD3	1.79	0.41
1:E:117:ILE:C	1:E:119:LYS:H	2.28	0.41
1:E:288:ILE:HG21	1:E:288:ILE:HD13	1.75	0.41
1:E:317:GLY:C	1:E:319:ASP:H	2.29	0.41
1:E:369:VAL:HG12	1:E:390:PHE:CE1	2.55	0.41
1:F:193:MET:HE2	1:F:193:MET:HB3	1.82	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:B:239:PRO:HB3	1:B:241:HIS:NE2	2.35	0.41
1:C:89:LEU:CD2	1:C:246:LEU:HD11	2.51	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: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:E:294:LYS:HA	1:E:294:LYS:HD2	1.90	0.41
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:268:GLU:C	1:G:270:PHE:N	2.79	0.41
1:G:284:VAL:HB	1:G:288:ILE:HB	2.03	0.41
1:H:37:ASP:HB2	1:H:258:LYS:HE2	2.03	0.41
1:H:191:LEU:HD22	1:H:193:MET:HE2	2.01	0.41
1:H:203:LYS:HD2	1:H:399:TYR:CD1	2.56	0.41
1:H:282:ILE:HG13	1:H:306:LEU:HD11	2.02	0.41
1:H:342:THR:CG2	1:H:396:MET:H	2.34	0.41
1:B:191:LEU:HD13	1:B:193:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD12	1:F:292:LEU:HA	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:A:291:TYR:CD1	1:A:291:TYR:C	2.99	0.40
1:B:29:LEU:HA	1:B:29:LEU:HD23	1.84	0.40
1:C:205:VAL:HG11	1:C:342:THR:CG2	2.51	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:83:ILE:HD13	1:B:261:MET:HE3	2.03	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
1:F:114:HIS:CE1	1:F:194:THR:HG1	2.38	0.40
1:H:107:THR:HG23	1:H:110:GLU:CD	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/546 (68%)	329 (89%)	29 (8%)	13 (4%)	3	13
1	B	401/546 (73%)	352 (88%)	28 (7%)	21 (5%)	1	8
1	C	405/546 (74%)	359 (89%)	27 (7%)	19 (5%)	2	9
1	D	438/546 (80%)	374 (85%)	44 (10%)	20 (5%)	2	9
1	E	394/546 (72%)	349 (89%)	31 (8%)	14 (4%)	2	12
1	F	413/546 (76%)	362 (88%)	36 (9%)	15 (4%)	2	12
1	G	395/546 (72%)	339 (86%)	35 (9%)	21 (5%)	1	7
1	H	396/546 (72%)	345 (87%)	36 (9%)	15 (4%)	2	12
All	All	3213/4368 (74%)	2809 (87%)	266 (8%)	138 (4%)	2	10

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	312 (95%)	16 (5%)	22	50
1	B	352/471 (75%)	337 (96%)	15 (4%)	26	53
1	C	355/471 (75%)	339 (96%)	16 (4%)	24	52
1	D	384/471 (82%)	362 (94%)	22 (6%)	18	45
1	E	345/471 (73%)	327 (95%)	18 (5%)	21	48
1	F	361/471 (77%)	344 (95%)	17 (5%)	23	51
1	G	348/471 (74%)	328 (94%)	20 (6%)	18	45
1	H	347/471 (74%)	324 (93%)	23 (7%)	15	40
All	All	2820/3768 (75%)	2673 (95%)	147 (5%)	21	48

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	44	THR
1	A	107	THR
1	A	115	LEU
1	A	201	LEU
1	A	203	LYS
1	A	223	ILE
1	A	284	VAL
1	A	307	THR
1	A	309	ILE
1	A	326	LYS
1	A	334	LEU
1	A	347	ILE
1	A	348	LEU
1	A	395	LEU
1	A	408	ASP
1	B	23	LEU
1	B	24	GLN
1	B	39	ILE
1	B	47	VAL
1	B	165	VAL
1	B	182	GLU
1	B	226	THR

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Mol	Chain	Res	Type
1	B	237	ILE
1	B	265	PHE
1	B	333	ILE
1	B	339	LEU
1	B	340	THR
1	B	347	ILE
1	B	348	LEU
1	B	401	ASN
1	C	6	ILE
1	C	23	LEU
1	C	203	LYS
1	C	223	ILE
1	C	226	THR
1	C	237	ILE
1	C	284	VAL
1	C	330	VAL
1	C	353	ARG
1	C	357	LYS
1	C	360	ILE
1	C	372	ILE
1	C	397	LYS
1	C	402	ASN
1	C	410	LEU
1	C	421	LEU
1	D	5	ASN
1	D	7	VAL
1	D	83	ILE
1	D	122	LEU
1	D	141	ASP
1	D	165	VAL
1	D	167	ARG
1	D	194	THR
1	D	198	THR
1	D	217	VAL
1	D	266	GLU
1	D	268	GLU
1	D	284	VAL
1	D	292	LEU
1	D	324	VAL
1	D	383	ARG
1	D	397	LYS
1	D	412	LYS

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Mol	Chain	Res	Type
1	D	413	ASP
1	D	421	LEU
1	D	439	LEU
1	D	441	LYS
1	E	7	VAL
1	E	72	ASN
1	E	141	ASP
1	E	165	VAL
1	E	226	THR
1	E	263	LYS
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	327	ARG
1	E	330	VAL
1	E	356	LYS
1	E	360	ILE
1	E	413	ASP
1	F	6	ILE
1	F	11	ARG
1	F	16	VAL
1	F	72	ASN
1	F	151	SER
1	F	165	VAL
1	F	186	LEU
1	F	220	SER
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	360	ILE
1	F	372	ILE
1	F	380	LEU
1	G	115	LEU
1	G	135	LYS
1	G	165	VAL

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Mol	Chain	Res	Type
1	G	201	LEU
1	G	268	GLU
1	G	292	LEU
1	G	309	ILE
1	G	326	LYS
1	G	328	LEU
1	G	339	LEU
1	G	347	ILE
1	G	371	VAL
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	35	ILE
1	H	37	ASP
1	H	107	THR
1	H	115	LEU
1	H	135	LYS
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	290	VAL
1	H	326	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	171	HIS
1	A	242	HIS
1	A	393	GLN
1	A	404	GLN
1	B	43	HIS
1	B	95	GLN
1	C	114	HIS
1	C	331	HIS
1	C	400	HIS
1	D	5	ASN
1	D	43	HIS
1	E	8	ASN
1	E	27	GLN
1	E	242	HIS
1	E	275	GLN
1	E	351	ASN
1	F	8	ASN
1	F	335	GLN
1	G	27	GLN
1	G	139	HIS
1	G	335	GLN
1	G	393	GLN
1	H	8	ASN
1	H	27	GLN
1	H	171	HIS
1	H	368	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	377/546 (69%)	0.05	9 (2%) 59 37	49, 71, 150, 244	0
1	B	405/546 (74%)	0.25	23 (5%) 29 15	43, 86, 182, 250	0
1	C	409/546 (74%)	0.12	14 (3%) 48 27	50, 76, 169, 239	0
1	D	442/546 (80%)	0.14	22 (4%) 34 17	41, 68, 155, 256	0
1	E	398/546 (72%)	0.17	11 (2%) 55 32	58, 84, 179, 239	0
1	F	417/546 (76%)	0.08	18 (4%) 40 21	45, 72, 160, 221	0
1	G	401/546 (73%)	0.22	18 (4%) 38 20	30, 74, 163, 223	0
1	H	400/546 (73%)	0.13	14 (3%) 47 26	50, 74, 170, 260	0
All	All	3249/4368 (74%)	0.15	129 (3%) 42 23	30, 77, 170, 260	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	TYR	7.1
1	D	429	PHE	5.3
1	F	423	TYR	5.2
1	G	372	ILE	4.8
1	D	384	GLU	4.7
1	C	361	GLY	4.7
1	B	343	CYS	4.3
1	G	363	PRO	4.2
1	D	312	GLY	4.0
1	H	337	TYR	3.9
1	H	361	GLY	3.9
1	H	359	ALA	3.8
1	A	349	SER	3.8
1	G	373	ASP	3.6
1	H	360	ILE	3.5
1	A	402	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	430	ILE	3.5
1	G	270	PHE	3.4
1	H	345	ALA	3.3
1	H	317	GLY	3.3
1	F	340	THR	3.2
1	C	342	THR	3.2
1	G	272	LYS	3.1
1	B	347	ILE	3.1
1	F	335	GLN	3.1
1	G	296	PRO	3.0
1	D	428	ARG	3.0
1	G	8	ASN	3.0
1	B	379	ALA	2.9
1	G	380	LEU	2.9
1	B	342	THR	2.9
1	G	418	THR	2.9
1	G	269	PHE	2.9
1	C	201	LEU	2.9
1	F	360	ILE	2.9
1	B	312	GLY	2.9
1	B	401	ASN	2.8
1	A	228	ILE	2.8
1	B	237	ILE	2.8
1	B	380	LEU	2.8
1	F	361	GLY	2.8
1	G	271	LEU	2.8
1	H	390	PHE	2.8
1	F	350	PRO	2.8
1	D	228	ILE	2.8
1	B	200	GLY	2.8
1	D	436	LEU	2.8
1	D	337	TYR	2.7
1	D	433	VAL	2.7
1	B	337	TYR	2.7
1	F	265	PHE	2.7
1	A	313	GLY	2.7
1	C	381	GLY	2.6
1	F	266	GLU	2.6
1	B	11	ARG	2.6
1	A	401	ASN	2.6
1	F	426	GLU	2.6
1	G	371	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	313	GLY	2.6
1	F	312	GLY	2.6
1	D	321	ALA	2.6
1	G	7	VAL	2.6
1	A	315	PRO	2.5
1	D	431	TYR	2.5
1	G	390	PHE	2.5
1	F	331	HIS	2.5
1	G	421	LEU	2.5
1	F	424	TYR	2.5
1	F	372	ILE	2.4
1	D	342	THR	2.4
1	C	202	PRO	2.4
1	E	337	TYR	2.4
1	F	337	TYR	2.4
1	D	435	ARG	2.4
1	B	280	ALA	2.4
1	B	314	SER	2.4
1	C	194	THR	2.3
1	E	338	GLY	2.3
1	D	335	GLN	2.3
1	E	359	ALA	2.3
1	A	348	LEU	2.3
1	C	334	LEU	2.3
1	F	339	LEU	2.3
1	B	315	PRO	2.3
1	C	200	GLY	2.3
1	F	313	GLY	2.3
1	B	228	ILE	2.3
1	E	388	ILE	2.3
1	G	280	ALA	2.3
1	C	322	ASP	2.3
1	E	336	GLY	2.3
1	E	368	GLN	2.2
1	E	194	THR	2.2
1	B	296	PRO	2.2
1	H	358	GLY	2.2
1	H	399	TYR	2.2
1	C	228	ILE	2.2
1	B	338	GLY	2.2
1	C	265	PHE	2.2
1	B	344	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	360	ILE	2.2
1	F	421	LEU	2.2
1	D	291	TYR	2.1
1	C	6	ILE	2.1
1	A	334	LEU	2.1
1	F	316	LEU	2.1
1	B	381	GLY	2.1
1	B	270	PHE	2.1
1	H	362	THR	2.1
1	H	424	TYR	2.1
1	B	408	ASP	2.1
1	H	413	ASP	2.1
1	H	415	TRP	2.1
1	D	298	VAL	2.1
1	A	235	LEU	2.1
1	D	237	ILE	2.1
1	G	228	ILE	2.1
1	D	199	THR	2.1
1	E	312	GLY	2.1
1	E	361	GLY	2.1
1	D	265	PHE	2.1
1	E	265	PHE	2.1
1	D	314	SER	2.1
1	H	417	HIS	2.1
1	G	382	PRO	2.1
1	E	313	GLY	2.0
1	B	201	LEU	2.0
1	D	373	ASP	2.0
1	D	388	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.