



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:57 PM UTC

PDB ID : 6AC3 / pdb_00006ac3
Title : Structure of a natural red emitting luciferase from Phrixothrix hirtus (P3121 crystal form)
Authors : Carrasco-Lopez, C.; Panjekar, S.; Naumov, P.; Rabeh, W.
Deposited on : 2018-07-24
Resolution : 3.60 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

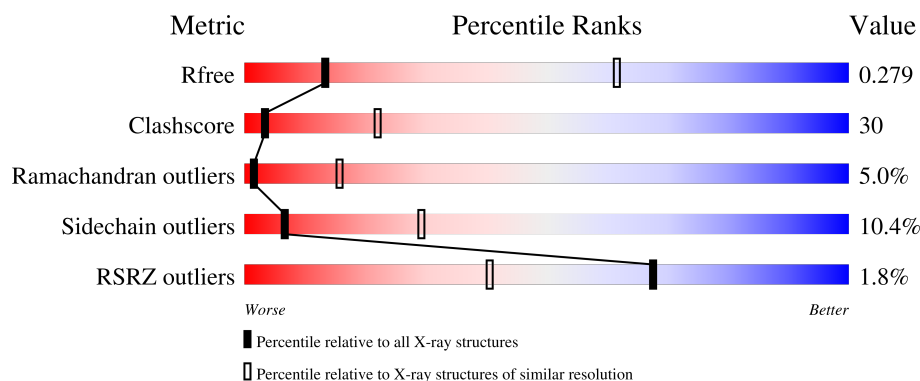
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	% 39% 30% 7% • 23%
1	B	546	3% 41% 41% 13% • •
1	C	546	% 39% 31% 6% • 24%
1	D	546	% 43% 27% 5% • 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13982 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.

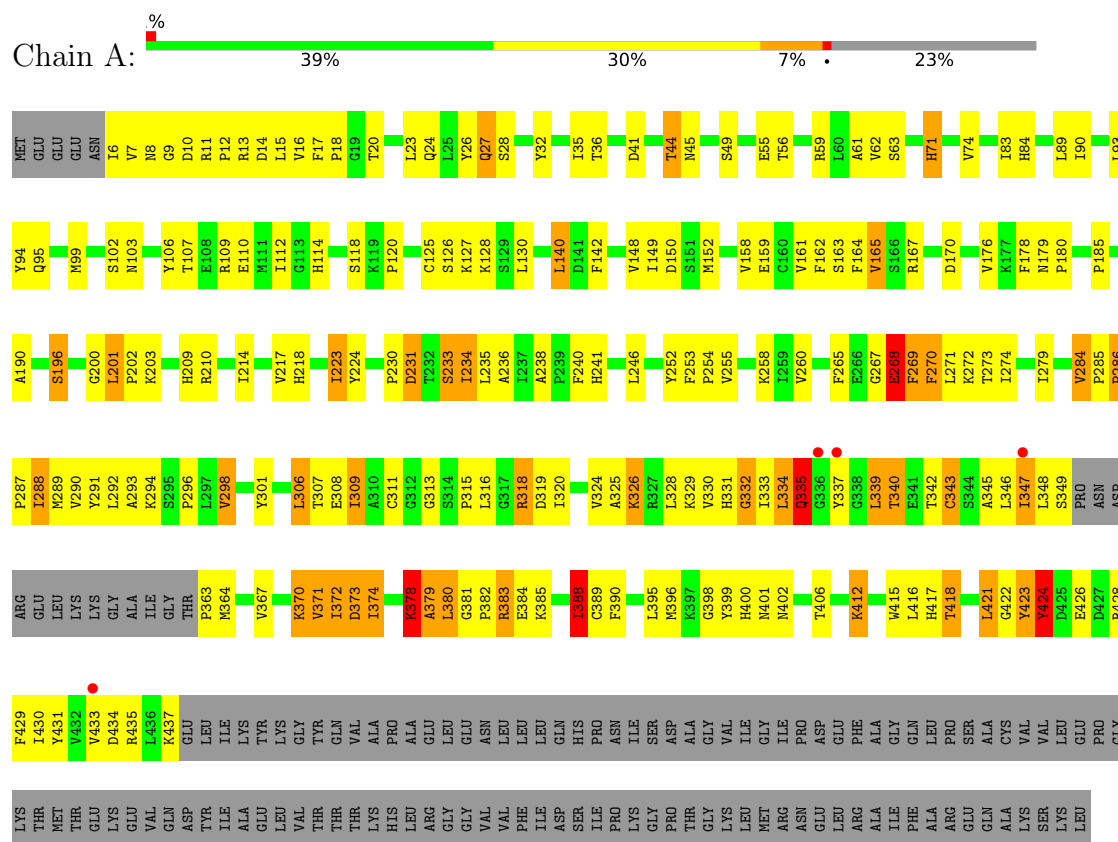
- Molecule 1 is a protein called Red-bioluminescence eliciting luciferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3296	2134	544	599	19			
1	B	528	Total	C	N	O	S	0	0	0
			4135	2667	686	760	22			
1	C	417	Total	C	N	O	S	0	0	0
			3279	2122	541	597	19			
1	D	416	Total	C	N	O	S	0	0	0
			3272	2117	540	596	19			

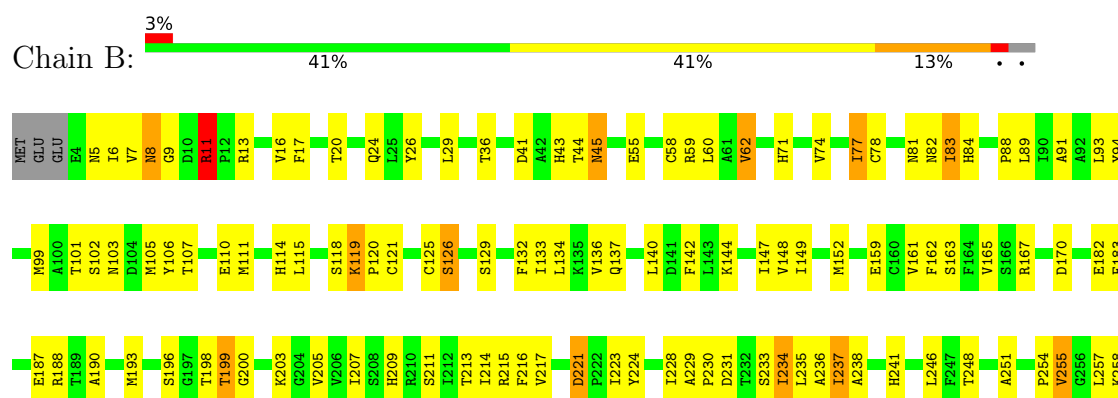
3 Residue-property plots [i](#)

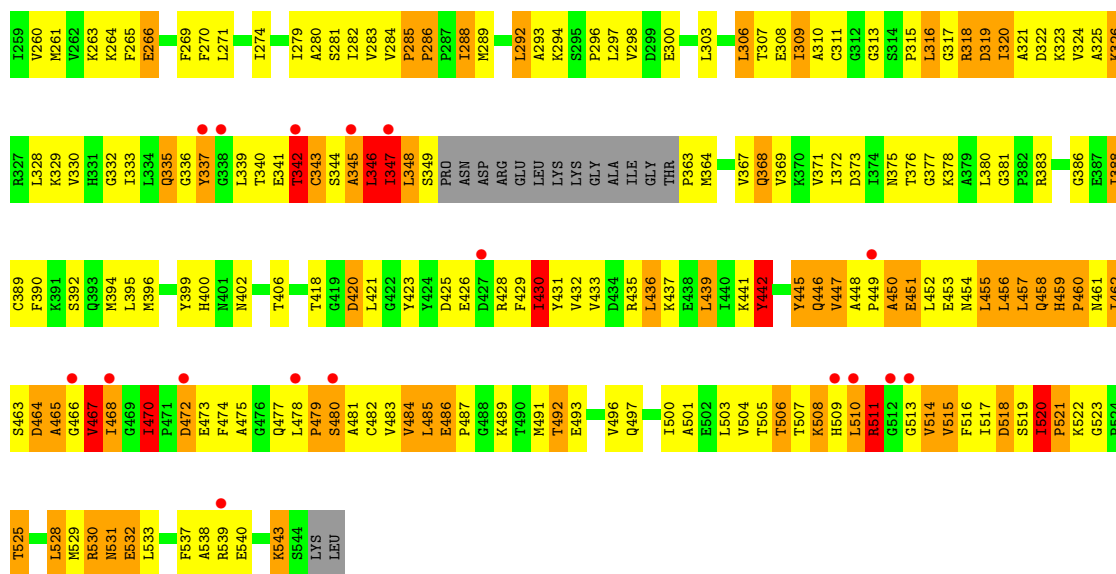
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Red-bioluminescence eliciting luciferase

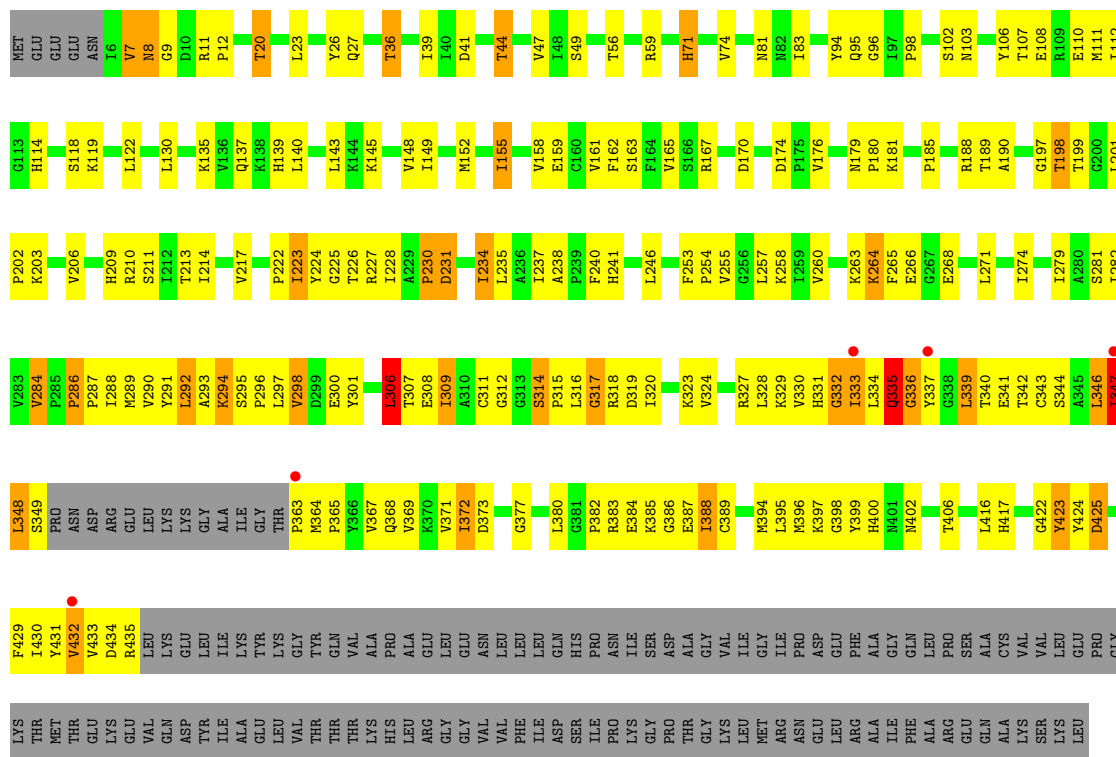


• Molecule 1: Red-bioluminescence eliciting luciferase

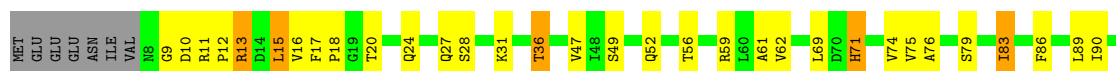
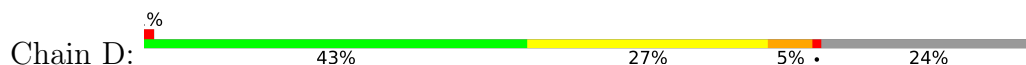




• Molecule 1: Red-bioluminescence eliciting luciferase



• Molecule 1: Red-bioluminescence eliciting luciferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.10Å 119.10Å 351.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.85 – 3.60 19.85 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.85-3.60) 98.4 (19.85-3.60)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.207 , 0.271 0.227 , 0.279	Depositor DCC
R_{free} test set	1020 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	97.3	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13982	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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	0.79	0/3375	1.24	22/4573 (0.5%)
1	B	0.78	0/4229	1.16	29/5730 (0.5%)
1	C	0.73	0/3358	1.15	22/4551 (0.5%)
1	D	0.74	0/3351	1.15	16/4541 (0.4%)
All	All	0.76	0/14313	1.17	89/19395 (0.5%)

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	3

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	VAL	N-CA-C	-10.48	102.21	112.17
1	D	270	PHE	N-CA-C	-9.55	100.82	111.14
1	A	435	ARG	N-CA-C	8.54	120.67	111.36
1	D	286	PRO	N-CA-C	7.76	120.16	110.70
1	C	286	PRO	N-CA-C	7.73	120.14	110.70
1	A	270	PHE	N-CA-C	-7.59	102.94	111.14
1	C	119	LYS	CA-C-N	7.51	128.10	119.99
1	C	119	LYS	C-N-CA	7.51	128.10	119.99
1	A	340	THR	N-CA-C	7.47	118.47	108.38
1	A	424	TYR	CA-CB-CG	7.38	127.18	113.90
1	B	348	LEU	N-CA-C	7.33	121.02	109.81
1	B	470	ILE	CA-C-N	7.26	127.26	119.28
1	B	470	ILE	C-N-CA	7.26	127.26	119.28
1	C	7	VAL	N-CA-C	-7.16	106.02	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	LEU	CA-C-N	7.16	130.35	121.83
1	A	421	LEU	C-N-CA	7.16	130.35	121.83
1	C	432	VAL	N-CA-C	6.92	117.83	107.80
1	A	10	ASP	N-CA-C	6.77	119.82	110.35
1	A	238	ALA	CA-C-N	6.71	128.22	119.84
1	A	238	ALA	C-N-CA	6.71	128.22	119.84
1	A	423	TYR	CA-C-N	-6.68	108.78	121.54
1	A	423	TYR	C-N-CA	-6.68	108.78	121.54
1	B	286	PRO	N-CA-C	6.54	118.67	110.70
1	B	450	ALA	O-C-N	6.49	125.64	120.83
1	D	119	LYS	CA-C-N	6.45	126.96	119.99
1	D	119	LYS	C-N-CA	6.45	126.96	119.99
1	C	423	TYR	N-CA-C	6.38	118.84	108.76
1	B	238	ALA	CA-C-N	6.30	127.72	119.84
1	B	238	ALA	C-N-CA	6.30	127.72	119.84
1	B	285	PRO	CA-C-N	6.29	126.86	120.38
1	B	285	PRO	C-N-CA	6.29	126.86	120.38
1	B	480	SER	CA-C-N	6.16	132.18	122.94
1	B	480	SER	C-N-CA	6.16	132.18	122.94
1	B	255	VAL	N-CA-C	-6.01	107.13	112.90
1	B	269	PHE	N-CA-C	-6.01	104.80	111.71
1	A	371	VAL	N-CA-C	5.97	117.14	112.12
1	B	136	VAL	N-CA-C	5.97	117.43	110.62
1	A	388	ILE	N-CA-C	5.92	116.71	108.89
1	B	346	LEU	CB-CA-C	-5.91	103.67	111.42
1	C	340	THR	N-CA-C	5.91	117.20	108.86
1	B	520	ILE	CA-C-N	-5.89	112.47	119.84
1	B	520	ILE	C-N-CA	-5.89	112.47	119.84
1	C	306	LEU	N-CA-C	5.88	117.87	108.41
1	C	298	VAL	N-CA-C	-5.85	106.62	112.17
1	B	306	LEU	N-CA-C	5.84	118.72	108.56
1	D	201	LEU	CA-C-N	-5.82	112.56	119.84
1	D	201	LEU	C-N-CA	-5.82	112.56	119.84
1	C	174	ASP	CA-C-N	5.81	125.48	119.56
1	C	174	ASP	C-N-CA	5.81	125.48	119.56
1	D	335	GLN	CA-C-N	5.79	132.75	121.41
1	D	335	GLN	C-N-CA	5.79	132.75	121.41
1	B	464	ASP	N-CA-C	5.74	119.03	111.28
1	B	430	ILE	N-CA-C	5.72	121.25	109.34
1	B	347	ILE	N-CA-C	5.71	121.23	109.34
1	D	397	LYS	N-CA-C	-5.69	106.38	113.15
1	A	286	PRO	N-CA-C	5.64	117.58	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	83	ILE	N-CA-C	5.62	121.03	109.34
1	A	412	LYS	N-CA-C	5.59	118.09	111.33
1	A	233	SER	N-CA-C	5.54	117.76	108.73
1	B	445	TYR	CA-C-N	5.52	132.08	121.54
1	B	445	TYR	C-N-CA	5.52	132.08	121.54
1	C	388	ILE	N-CA-C	5.52	116.17	108.89
1	B	474	PHE	N-CA-C	-5.51	106.40	113.01
1	C	264	LYS	CA-C-N	5.47	129.35	120.60
1	C	264	LYS	C-N-CA	5.47	129.35	120.60
1	B	518	ASP	N-CA-C	5.46	119.91	111.56
1	B	317	GLY	N-CA-C	-5.38	106.89	115.66
1	A	201	LEU	CA-C-N	-5.35	113.15	119.84
1	A	201	LEU	C-N-CA	-5.35	113.15	119.84
1	B	442	TYR	N-CA-C	5.34	122.18	110.80
1	A	13	ARG	N-CA-C	-5.31	105.94	112.90
1	D	152	MET	N-CA-C	-5.29	106.99	113.50
1	C	238	ALA	CA-C-N	5.28	126.44	119.84
1	C	238	ALA	C-N-CA	5.28	126.44	119.84
1	C	155	ILE	N-CA-C	5.28	113.97	106.53
1	C	314	SER	CA-C-N	5.27	126.43	119.84
1	C	314	SER	C-N-CA	5.27	126.43	119.84
1	C	397	LYS	N-CA-C	-5.25	106.90	113.15
1	D	381	GLY	CA-C-N	5.17	125.15	120.03
1	D	381	GLY	C-N-CA	5.17	125.15	120.03
1	D	221	ASP	CA-C-N	5.12	126.13	120.45
1	D	221	ASP	C-N-CA	5.12	126.13	120.45
1	C	335	GLN	CA-C-N	5.04	131.28	121.41
1	C	335	GLN	C-N-CA	5.04	131.28	121.41
1	A	273	THR	N-CA-C	5.03	116.45	111.07
1	B	221	ASP	CA-C-N	5.03	125.47	120.04
1	B	221	ASP	C-N-CA	5.03	125.47	120.04
1	A	370	LYS	N-CA-C	5.02	116.31	109.18
1	D	390	PHE	N-CA-C	5.01	117.73	109.72

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	11	ARG	Sidechain
1	B	511	ARG	Sidechain
1	B	539	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	3296	0	3330	219	0
1	B	4135	0	4187	306	0
1	C	3279	0	3306	171	0
1	D	3272	0	3297	166	0
All	All	13982	0	14120	849	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 30.

All (849) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLY:CA	1:B:348:LEU:HB3	1.41	1.46
1:A:9:GLY:CA	1:A:363:PRO:HG2	1.57	1.34
1:B:347:ILE:HD12	1:B:390:PHE:CE2	1.68	1.28
1:B:347:ILE:CD1	1:B:390:PHE:HE2	1.48	1.26
1:C:339:LEU:HD23	1:C:344:SER:CB	1.69	1.23
1:C:339:LEU:CD2	1:C:344:SER:HB3	1.72	1.20
1:D:372:ILE:O	1:D:380:LEU:HD23	1.36	1.19
1:B:342:THR:CG2	1:B:396:MET:HB3	1.74	1.17
1:C:364:MET:CG	1:C:365:PRO:HD2	1.74	1.16
1:B:342:THR:HG21	1:B:396:MET:HB3	1.29	1.14
1:C:364:MET:HG2	1:C:365:PRO:HD2	1.15	1.13
1:B:342:THR:HG21	1:B:396:MET:CB	1.78	1.13
1:B:336:GLY:HA2	1:B:348:LEU:CB	1.78	1.12
1:B:468:ILE:HG21	1:B:533:LEU:HB2	1.27	1.12
1:B:517:ILE:HG13	1:B:518:ASP:H	1.01	1.11
1:A:9:GLY:CA	1:A:363:PRO:CG	2.28	1.10
1:A:9:GLY:HA2	1:A:363:PRO:CG	1.81	1.10
1:C:339:LEU:HD23	1:C:344:SER:HB3	1.12	1.09
1:A:378:LYS:HE2	1:A:378:LYS:HA	1.32	1.07
1:C:364:MET:CG	1:C:365:PRO:CD	2.32	1.07
1:C:347:ILE:HB	1:C:363:PRO:N	1.68	1.06
1:C:364:MET:HG2	1:C:365:PRO:CD	1.85	1.05
1:B:336:GLY:CA	1:B:348:LEU:CB	2.33	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLY:HA3	1:B:348:LEU:HB3	1.35	1.02
1:B:347:ILE:HD12	1:B:390:PHE:HE2	0.85	1.02
1:B:336:GLY:HA2	1:B:348:LEU:HB3	1.03	1.01
1:A:347:ILE:HG12	1:A:363:PRO:HA	1.44	0.99
1:B:470:ILE:HD12	1:B:478:LEU:HB3	1.44	0.99
1:A:9:GLY:HA2	1:A:363:PRO:HG2	1.00	0.98
1:A:380:LEU:HD23	1:A:385:LYS:O	1.63	0.98
1:B:347:ILE:HG22	1:B:347:ILE:O	1.61	0.98
1:B:497:GLN:HG3	1:B:510:LEU:HD11	1.43	0.98
1:B:510:LEU:HD13	1:B:514:VAL:HG23	1.47	0.97
1:D:13:ARG:NH1	1:D:221:ASP:OD2	1.97	0.96
1:D:399:TYR:H	1:D:406:THR:HG22	1.28	0.96
1:B:346:LEU:O	1:B:347:ILE:HB	1.66	0.96
1:A:311:CYS:H	1:A:335:GLN:HG2	1.27	0.96
1:B:470:ILE:HD11	1:B:480:SER:HB2	1.47	0.96
1:B:497:GLN:HG3	1:B:510:LEU:CD1	1.94	0.96
1:B:510:LEU:CD1	1:B:514:VAL:HG23	1.96	0.96
1:B:342:THR:HG21	1:B:396:MET:CA	1.96	0.95
1:B:347:ILE:CD1	1:B:390:PHE:CE2	2.38	0.94
1:A:334:LEU:O	1:A:335:GLN:HG3	1.66	0.94
1:B:472:ASP:O	1:B:478:LEU:HD13	1.67	0.93
1:C:348:LEU:HD12	1:C:364:MET:HE1	1.51	0.93
1:B:479:PRO:HD2	1:B:511:ARG:HB2	1.51	0.92
1:C:237:ILE:HD11	1:C:265:PHE:HA	1.54	0.90
1:C:364:MET:HG3	1:C:365:PRO:CD	2.02	0.89
1:A:9:GLY:HA3	1:A:363:PRO:HG2	1.53	0.89
1:B:517:ILE:HG13	1:B:518:ASP:N	1.83	0.89
1:C:348:LEU:CD1	1:C:364:MET:HE1	2.03	0.89
1:A:339:LEU:HB3	1:A:345:ALA:H	1.38	0.89
1:A:382:PRO:HA	1:A:424:TYR:HD1	1.35	0.89
1:B:480:SER:OG	1:B:537:PHE:CZ	2.27	0.88
1:D:347:ILE:HG12	1:D:363:PRO:HA	1.56	0.87
1:B:517:ILE:CG1	1:B:518:ASP:H	1.88	0.87
1:B:468:ILE:CG2	1:B:533:LEU:HB2	2.04	0.87
1:C:107:THR:HG23	1:C:110:GLU:H	1.40	0.87
1:C:347:ILE:CB	1:C:363:PRO:N	2.37	0.87
1:C:399:TYR:H	1:C:406:THR:HG22	1.40	0.86
1:A:423:TYR:O	1:A:424:TYR:CB	2.19	0.86
1:B:517:ILE:HD13	1:B:540:GLU:OE2	1.75	0.86
1:A:9:GLY:HA3	1:A:363:PRO:CG	2.04	0.84
1:B:496:VAL:HB	1:B:514:VAL:HG21	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ILE:HA	1:C:363:PRO:N	1.91	0.84
1:D:372:ILE:O	1:D:380:LEU:CD2	2.23	0.84
1:B:504:VAL:HB	1:B:508:LYS:HD3	1.60	0.84
1:A:385:LYS:HA	1:A:422:GLY:O	1.77	0.84
1:A:342:THR:HG22	1:A:343:CYS:H	1.44	0.82
1:A:423:TYR:O	1:A:424:TYR:O	1.98	0.81
1:D:337:TYR:CE2	1:D:348:LEU:HA	2.15	0.81
1:D:347:ILE:O	1:D:347:ILE:HG22	1.79	0.81
1:B:335:GLN:O	1:B:348:LEU:HB2	1.80	0.81
1:A:311:CYS:N	1:A:335:GLN:HG2	1.95	0.81
1:D:346:LEU:O	1:D:347:ILE:HB	1.81	0.80
1:C:348:LEU:HD12	1:C:364:MET:CE	2.11	0.80
1:D:13:ARG:HG3	1:D:221:ASP:OD2	1.82	0.80
1:A:382:PRO:HA	1:A:424:TYR:CD1	2.15	0.80
1:A:423:TYR:O	1:A:424:TYR:HB3	1.80	0.80
1:B:342:THR:CG2	1:B:396:MET:CB	2.47	0.79
1:A:334:LEU:C	1:A:335:GLN:HG3	2.07	0.79
1:A:380:LEU:CD2	1:A:385:LYS:O	2.31	0.79
1:D:13:ARG:HH11	1:D:221:ASP:CG	1.91	0.78
1:A:372:ILE:O	1:A:380:LEU:HD13	1.84	0.78
1:A:399:TYR:H	1:A:406:THR:HG22	1.47	0.78
1:B:335:GLN:C	1:B:348:LEU:HB2	2.09	0.78
1:D:13:ARG:HD2	1:D:222:PRO:HD2	1.65	0.78
1:B:441:LYS:HE2	1:B:530:ARG:HB3	1.66	0.77
1:B:429:PHE:O	1:B:431:TYR:N	2.18	0.77
1:C:364:MET:HG3	1:C:365:PRO:HD3	1.66	0.77
1:B:436:LEU:CD1	1:B:450:ALA:H	1.97	0.77
1:D:347:ILE:CD1	1:D:390:PHE:CE1	2.67	0.77
1:C:342:THR:HG22	1:C:343:CYS:H	1.50	0.77
1:A:347:ILE:HG23	1:A:363:PRO:N	2.00	0.76
1:A:268:GLU:C	1:A:270:PHE:H	1.91	0.76
1:A:307:THR:HG22	1:A:308:GLU:HG3	1.66	0.76
1:C:347:ILE:HG12	1:C:347:ILE:O	1.83	0.76
1:C:429:PHE:HB3	1:C:431:TYR:CE2	2.20	0.76
1:B:346:LEU:O	1:B:347:ILE:CB	2.33	0.76
1:A:378:LYS:HA	1:A:378:LYS:CE	2.03	0.76
1:A:103:ASN:HD22	1:A:241:HIS:CE1	2.04	0.75
1:B:529:MET:HB2	1:B:532:GLU:HB2	1.67	0.75
1:B:453:GLU:O	1:B:457:LEU:HB2	1.86	0.75
1:C:289:MET:HE3	1:C:311:CYS:HB2	1.69	0.75
1:D:347:ILE:CG2	1:D:432:VAL:HG21	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:LEU:HG	1:B:511:ARG:HB3	1.70	0.74
1:A:337:TYR:HD2	1:A:348:LEU:HA	1.52	0.74
1:C:364:MET:HG3	1:C:365:PRO:HD2	1.66	0.74
1:D:174:ASP:HB3	1:D:177:LYS:HD3	1.70	0.74
1:D:89:LEU:HA	1:D:99:MET:HE3	1.70	0.73
1:B:125:CYS:SG	1:B:129:SER:HB2	2.28	0.73
1:A:9:GLY:HA3	1:A:363:PRO:CB	2.18	0.73
1:C:347:ILE:HG22	1:C:363:PRO:HA	1.69	0.73
1:A:268:GLU:HA	1:A:271:LEU:HD23	1.71	0.73
1:A:334:LEU:HB3	1:A:349:SER:HB3	1.70	0.73
1:A:9:GLY:HA3	1:A:363:PRO:HB2	1.69	0.73
1:D:268:GLU:N	1:D:268:GLU:OE1	2.20	0.73
1:D:140:LEU:HB3	1:D:142:PHE:CE1	2.24	0.72
1:B:342:THR:HG23	1:B:396:MET:HB3	1.67	0.72
1:A:378:LYS:HE2	1:A:378:LYS:CA	2.18	0.72
1:D:268:GLU:O	1:D:270:PHE:N	2.21	0.72
1:B:458:GLN:O	1:B:459:HIS:ND1	2.18	0.72
1:B:480:SER:OG	1:B:537:PHE:CE1	2.41	0.72
1:B:347:ILE:H	1:B:364:MET:HG3	1.53	0.71
1:B:255:VAL:HG23	1:B:257:LEU:HG	1.72	0.71
1:D:268:GLU:C	1:D:270:PHE:H	1.98	0.71
1:A:236:ALA:HB2	1:A:252:TYR:HE2	1.56	0.71
1:A:285:PRO:HD2	1:A:288:ILE:HD11	1.73	0.71
1:B:451:GLU:OE2	1:B:467:VAL:HG23	1.91	0.71
1:B:468:ILE:HG21	1:B:533:LEU:CB	2.15	0.71
1:B:497:GLN:CG	1:B:510:LEU:CD1	2.67	0.71
1:B:347:ILE:O	1:B:347:ILE:CG2	2.35	0.70
1:B:472:ASP:C	1:B:478:LEU:HD13	2.16	0.70
1:C:348:LEU:CD1	1:C:364:MET:CE	2.69	0.70
1:A:372:ILE:O	1:A:373:ASP:CB	2.38	0.70
1:B:463:SER:HB3	1:B:483:VAL:HG13	1.73	0.70
1:C:339:LEU:HD21	1:C:344:SER:HB3	1.72	0.70
1:C:342:THR:HG21	1:C:395:LEU:HA	1.73	0.70
1:C:396:MET:HE3	1:C:416:LEU:HD11	1.73	0.70
1:B:11:ARG:CG	1:B:11:ARG:HH11	2.05	0.69
1:B:451:GLU:OE2	1:B:467:VAL:CG2	2.41	0.69
1:D:337:TYR:HE2	1:D:348:LEU:HA	1.55	0.69
1:A:389:CYS:HA	1:A:418:THR:OG1	1.92	0.69
1:B:235:LEU:HB3	1:B:282:ILE:HG22	1.75	0.68
1:A:334:LEU:O	1:A:335:GLN:CG	2.42	0.68
1:C:429:PHE:O	1:C:431:TYR:N	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:PRO:HD2	1:B:511:ARG:CB	2.22	0.68
1:B:510:LEU:HD13	1:B:514:VAL:H	1.59	0.68
1:A:55:GLU:OE2	1:A:59:ARG:HD2	1.93	0.68
1:B:497:GLN:HG3	1:B:510:LEU:HD12	1.76	0.68
1:B:140:LEU:HB3	1:B:142:PHE:CE1	2.29	0.67
1:C:103:ASN:HD22	1:C:241:HIS:CE1	2.12	0.67
1:A:6:ILE:HG22	1:A:6:ILE:O	1.94	0.67
1:A:383:ARG:HA	1:A:423:TYR:HD2	1.58	0.67
1:B:190:ALA:HB2	1:B:209:HIS:CD2	2.30	0.67
1:A:311:CYS:H	1:A:335:GLN:CG	2.02	0.67
1:B:149:ILE:HA	1:B:161:VAL:HG23	1.77	0.67
1:B:500:ILE:HG22	1:B:503:LEU:HD13	1.75	0.67
1:B:11:ARG:HH11	1:B:11:ARG:HG3	1.60	0.67
1:C:425:ASP:O	1:C:429:PHE:HB2	1.95	0.67
1:B:510:LEU:HD11	1:B:514:VAL:HG23	1.75	0.67
1:D:17:PHE:CD2	1:D:24:GLN:HB2	2.30	0.67
1:A:400:HIS:C	1:A:402:ASN:H	2.03	0.67
1:C:422:GLY:HA2	1:C:435:ARG:H	1.60	0.66
1:B:436:LEU:HD13	1:B:450:ALA:H	1.59	0.66
1:C:294:LYS:HE3	1:C:323:LYS:NZ	2.11	0.66
1:C:371:VAL:HG13	1:C:380:LEU:HB2	1.76	0.66
1:D:234:ILE:HD12	1:D:281:SER:HB3	1.77	0.66
1:B:286:PRO:HA	1:B:289:MET:HB2	1.75	0.66
1:B:464:ASP:HB2	1:B:484:VAL:HG13	1.77	0.66
1:D:347:ILE:HG22	1:D:432:VAL:HG21	1.76	0.66
1:A:334:LEU:C	1:A:335:GLN:CG	2.69	0.66
1:C:7:VAL:O	1:C:9:GLY:N	2.27	0.66
1:C:294:LYS:HE3	1:C:323:LYS:HZ3	1.61	0.66
1:D:372:ILE:HG22	1:D:379:ALA:N	2.11	0.66
1:A:429:PHE:O	1:A:431:TYR:N	2.26	0.65
1:B:316:LEU:HD21	1:B:525:THR:HG21	1.76	0.65
1:C:74:VAL:HG12	1:C:98:PRO:HB2	1.76	0.65
1:D:347:ILE:CG1	1:D:363:PRO:HA	2.25	0.65
1:D:380:LEU:HD12	1:D:384:GLU:OE2	1.95	0.65
1:D:429:PHE:O	1:D:431:TYR:N	2.28	0.65
1:A:342:THR:HG21	1:A:395:LEU:HA	1.79	0.65
1:A:318:ARG:O	1:A:320:ILE:N	2.30	0.65
1:C:317:GLY:O	1:C:320:ILE:N	2.29	0.65
1:A:230:PRO:O	1:A:231:ASP:HB2	1.96	0.65
1:A:347:ILE:HD12	1:A:390:PHE:CE1	2.31	0.65
1:C:197:GLY:O	1:C:199:THR:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:TYR:CD2	1:C:364:MET:HE2	2.32	0.65
1:C:268:GLU:HA	1:C:271:LEU:HD23	1.78	0.65
1:C:316:LEU:O	1:C:318:ARG:N	2.29	0.65
1:B:455:LEU:HD23	1:B:467:VAL:HG22	1.78	0.65
1:A:311:CYS:O	1:A:335:GLN:HB2	1.97	0.64
1:B:285:PRO:HD2	1:B:288:ILE:HD11	1.80	0.64
1:C:201:LEU:HD12	1:C:202:PRO:HD2	1.80	0.64
1:A:371:VAL:C	1:A:372:ILE:HG13	2.22	0.64
1:C:339:LEU:CD2	1:C:344:SER:CB	2.48	0.64
1:B:505:THR:HG22	1:B:506:THR:H	1.62	0.64
1:B:152:MET:HE1	1:B:162:PHE:CG	2.34	0.63
1:C:230:PRO:O	1:C:231:ASP:HB2	1.96	0.63
1:B:472:ASP:OD1	1:B:478:LEU:HD22	1.98	0.63
1:B:497:GLN:CG	1:B:510:LEU:HD12	2.27	0.63
1:D:347:ILE:HA	1:D:363:PRO:CA	2.28	0.63
1:D:429:PHE:HB3	1:D:431:TYR:CE2	2.34	0.63
1:B:342:THR:HG21	1:B:396:MET:HA	1.79	0.63
1:B:435:ARG:HH22	1:B:457:LEU:CD2	2.11	0.63
1:B:533:LEU:HD12	1:B:533:LEU:H	1.64	0.63
1:A:59:ARG:NH2	1:A:170:ASP:O	2.31	0.63
1:C:159:GLU:OE1	1:C:167:ARG:NH1	2.32	0.63
1:A:44:THR:O	1:A:45:ASN:HB2	1.99	0.62
1:B:59:ARG:NH2	1:B:170:ASP:O	2.31	0.62
1:B:44:THR:O	1:B:45:ASN:HB2	1.98	0.62
1:B:89:LEU:HA	1:B:99:MET:HE3	1.81	0.62
1:B:335:GLN:N	1:B:335:GLN:OE1	2.32	0.62
1:D:103:ASN:HD22	1:D:241:HIS:CE1	2.17	0.62
1:B:205:VAL:HG11	1:B:342:THR:HG23	1.80	0.62
1:B:347:ILE:HD11	1:B:390:PHE:CE2	2.34	0.62
1:A:7:VAL:O	1:A:9:GLY:N	2.33	0.62
1:B:510:LEU:HD13	1:B:514:VAL:CG2	2.26	0.62
1:A:125:CYS:O	1:A:149:ILE:HG12	2.00	0.61
1:C:339:LEU:HD23	1:C:344:SER:OG	1.99	0.61
1:A:26:TYR:HB2	1:A:94:TYR:CE1	2.35	0.61
1:B:470:ILE:N	1:B:478:LEU:O	2.31	0.61
1:B:439:LEU:HG	1:B:442:TYR:OH	2.00	0.61
1:C:312:GLY:HA2	1:C:339:LEU:HD11	1.82	0.61
1:B:296:PRO:HB2	1:B:297:LEU:HG	1.81	0.61
1:B:321:ALA:HA	1:B:333:ILE:HD11	1.80	0.61
1:D:325:ALA:HB2	1:D:333:ILE:HG22	1.83	0.61
1:A:27:GLN:HG2	1:D:15:LEU:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:MET:HE3	1:A:311:CYS:HB2	1.81	0.61
1:B:521:PRO:HG3	1:B:533:LEU:HD11	1.82	0.61
1:C:347:ILE:CA	1:C:363:PRO:N	2.62	0.61
1:D:346:LEU:O	1:D:347:ILE:CB	2.48	0.61
1:C:264:LYS:HD3	1:C:266:GLU:OE2	2.00	0.61
1:B:26:TYR:HB2	1:B:94:TYR:CE1	2.36	0.60
1:B:383:ARG:HA	1:B:423:TYR:CD2	2.35	0.60
1:B:293:ALA:HB2	1:B:324:VAL:HG13	1.83	0.60
1:D:291:TYR:O	1:D:295:SER:HB3	2.01	0.60
1:D:287:PRO:O	1:D:290:VAL:HG22	2.01	0.60
1:D:307:THR:HG22	1:D:308:GLU:HG3	1.82	0.60
1:D:74:VAL:HG11	1:D:118:SER:HB2	1.83	0.60
1:A:346:LEU:C	1:A:347:ILE:HG13	2.27	0.60
1:B:103:ASN:OD1	1:B:105:MET:N	2.34	0.60
1:B:529:MET:O	1:B:531:ASN:N	2.34	0.60
1:D:194:THR:HA	1:D:204:GLY:HA2	1.83	0.60
1:D:372:ILE:HG22	1:D:379:ALA:HA	1.82	0.60
1:B:347:ILE:HG21	1:B:432:VAL:CG2	2.31	0.60
1:D:9:GLY:HA3	1:D:363:PRO:HB2	1.84	0.60
1:C:425:ASP:OD2	1:C:433:VAL:HG13	2.00	0.60
1:A:400:HIS:O	1:A:402:ASN:N	2.34	0.60
1:B:458:GLN:O	1:B:458:GLN:NE2	2.35	0.59
1:D:372:ILE:HG22	1:D:379:ALA:CA	2.31	0.59
1:D:385:LYS:HA	1:D:422:GLY:O	2.03	0.59
1:A:371:VAL:HG11	1:A:384:GLU:O	2.02	0.59
1:A:333:ILE:C	1:A:334:LEU:HD13	2.27	0.59
1:D:274:ILE:HG13	1:D:279:ILE:HB	1.84	0.59
1:A:130:LEU:HD21	1:A:158:VAL:HG21	1.84	0.59
1:A:102:SER:HA	1:A:114:HIS:CE1	2.38	0.59
1:A:149:ILE:HA	1:A:161:VAL:HG23	1.85	0.59
1:A:293:ALA:HB2	1:A:324:VAL:HG13	1.84	0.59
1:B:11:ARG:NE	1:C:176:VAL:O	2.36	0.59
1:D:422:GLY:HA3	1:D:434:ASP:HA	1.85	0.59
1:D:237:ILE:HG12	1:D:262:VAL:HB	1.84	0.59
1:A:339:LEU:O	1:A:340:THR:HG23	2.03	0.59
1:B:207:ILE:CD1	1:B:342:THR:HG22	2.32	0.59
1:B:333:ILE:HG13	1:B:333:ILE:O	2.02	0.59
1:B:325:ALA:HA	1:B:330:VAL:HG12	1.85	0.59
1:D:338:GLY:O	1:D:339:LEU:O	2.21	0.58
1:D:399:TYR:N	1:D:406:THR:HG22	2.10	0.58
1:B:340:THR:HG21	1:B:395:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:THR:HG22	1:A:343:CYS:N	2.14	0.58
1:B:455:LEU:HD11	1:B:465:ALA:HA	1.84	0.58
1:C:106:TYR:HE2	1:C:114:HIS:ND1	2.00	0.58
1:C:348:LEU:HD11	1:C:364:MET:HE1	1.84	0.58
1:B:224:TYR:CD2	1:B:364:MET:HE3	2.39	0.58
1:B:347:ILE:HG12	1:B:363:PRO:HA	1.85	0.58
1:A:27:GLN:CD	1:D:15:LEU:CD1	2.76	0.58
1:B:26:TYR:HB2	1:B:94:TYR:HE1	1.68	0.58
1:B:320:ILE:O	1:B:324:VAL:HG22	2.04	0.58
1:C:152:MET:HE1	1:C:162:PHE:CD1	2.38	0.58
1:D:347:ILE:HD12	1:D:390:PHE:CE1	2.38	0.58
1:B:510:LEU:HD13	1:B:514:VAL:N	2.18	0.58
1:B:340:THR:HG21	1:B:395:LEU:CD2	2.34	0.58
1:C:311:CYS:O	1:C:335:GLN:NE2	2.32	0.58
1:B:340:THR:HG22	1:B:340:THR:O	2.04	0.57
1:A:372:ILE:O	1:A:373:ASP:HB3	2.03	0.57
1:A:337:TYR:HD2	1:A:348:LEU:CA	2.17	0.57
1:C:11:ARG:HG3	1:C:12:PRO:HD2	1.86	0.57
1:B:335:GLN:C	1:B:348:LEU:CB	2.78	0.57
1:C:228:ILE:HD11	1:C:307:THR:HG21	1.84	0.57
1:B:120:PRO:HD2	1:B:142:PHE:HE2	1.68	0.57
1:D:271:LEU:HD21	1:D:291:TYR:HE2	1.70	0.57
1:A:159:GLU:CD	1:A:167:ARG:HH11	2.12	0.57
1:B:483:VAL:O	1:B:516:PHE:HA	2.04	0.57
1:C:383:ARG:HA	1:C:423:TYR:CD2	2.40	0.57
1:C:425:ASP:OD2	1:C:433:VAL:HG22	2.05	0.57
1:B:373:ASP:HB3	1:B:375:ASN:H	1.69	0.57
1:D:339:LEU:HD23	1:D:344:SER:HB3	1.85	0.57
1:D:425:ASP:O	1:D:429:PHE:HB2	2.05	0.57
1:A:63:SER:HB3	1:A:164:PHE:CE2	2.40	0.57
1:C:287:PRO:O	1:C:290:VAL:HG22	2.05	0.57
1:C:307:THR:HG22	1:C:308:GLU:HG3	1.87	0.57
1:B:459:HIS:N	1:B:460:PRO:HD3	2.21	0.56
1:B:493:GLU:HA	1:B:514:VAL:HB	1.86	0.56
1:D:342:THR:HG22	1:D:343:CYS:H	1.68	0.56
1:A:27:GLN:HG3	1:D:13:ARG:O	2.05	0.56
1:A:311:CYS:HB3	1:A:335:GLN:NE2	2.20	0.56
1:C:274:ILE:HG13	1:C:279:ILE:HB	1.86	0.56
1:A:148:VAL:O	1:A:161:VAL:HG23	2.06	0.56
1:B:74:VAL:HG12	1:B:120:PRO:HB3	1.88	0.56
1:D:294:LYS:HD3	1:D:323:LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:SER:OG	1:A:254:PRO:HA	2.05	0.56
1:B:470:ILE:O	1:B:478:LEU:N	2.38	0.56
1:C:293:ALA:HB2	1:C:324:VAL:HG13	1.87	0.56
1:B:399:TYR:H	1:B:406:THR:HG22	1.69	0.56
1:A:268:GLU:O	1:A:270:PHE:N	2.33	0.56
1:A:384:GLU:N	1:A:423:TYR:HB2	2.21	0.56
1:A:429:PHE:HB3	1:A:431:TYR:CE1	2.41	0.56
1:B:373:ASP:HB2	1:B:377:GLY:H	1.71	0.56
1:A:114:HIS:C	1:A:114:HIS:CD2	2.84	0.56
1:C:296:PRO:O	1:C:298:VAL:HG13	2.05	0.56
1:B:207:ILE:HD11	1:B:342:THR:HG22	1.88	0.56
1:C:347:ILE:HG22	1:C:363:PRO:CA	2.36	0.56
1:D:59:ARG:NH1	1:D:173:PHE:HB3	2.20	0.56
1:B:309:ILE:HB	1:B:333:ILE:HG22	1.88	0.55
1:C:372:ILE:C	1:C:380:LEU:HD23	2.31	0.55
1:C:137:GLN:HB2	1:C:143:LEU:HD23	1.89	0.55
1:A:337:TYR:CD2	1:A:348:LEU:HA	2.38	0.55
1:A:423:TYR:O	1:A:424:TYR:HB2	2.05	0.55
1:C:148:VAL:O	1:C:161:VAL:HG23	2.06	0.55
1:C:314:SER:O	1:C:314:SER:OG	2.22	0.55
1:B:140:LEU:HD13	1:B:142:PHE:CZ	2.41	0.55
1:A:313:GLY:O	1:A:339:LEU:HD11	2.07	0.55
1:B:484:VAL:HG21	1:B:518:ASP:O	2.06	0.55
1:A:326:LYS:HE2	1:C:301:TYR:CE2	2.42	0.55
1:B:313:GLY:O	1:B:339:LEU:HD21	2.07	0.55
1:B:436:LEU:HD11	1:B:451:GLU:N	2.22	0.54
1:C:284:VAL:HB	1:C:288:ILE:HG13	1.89	0.54
1:D:316:LEU:HD23	1:D:317:GLY:H	1.71	0.54
1:B:473:GLU:N	1:B:478:LEU:HD13	2.22	0.54
1:A:27:GLN:CD	1:D:15:LEU:HD12	2.33	0.54
1:A:309:ILE:HG12	1:A:330:VAL:HG21	1.90	0.54
1:C:106:TYR:HB2	1:C:111:MET:HE2	1.89	0.54
1:C:240:PHE:O	1:C:246:LEU:HB2	2.07	0.54
1:C:286:PRO:HA	1:C:289:MET:HB2	1.89	0.54
1:C:347:ILE:HG13	1:C:432:VAL:HG21	1.90	0.54
1:D:399:TYR:H	1:D:406:THR:CG2	2.13	0.54
1:A:11:ARG:HG3	1:A:12:PRO:HD2	1.90	0.54
1:B:198:THR:O	1:B:203:LYS:NZ	2.40	0.54
1:C:203:LYS:HB3	1:C:399:TYR:HD2	1.73	0.54
1:C:422:GLY:HA3	1:C:434:ASP:HA	1.90	0.54
1:B:336:GLY:HA2	1:B:348:LEU:CA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:HIS:CD2	1:D:71:HIS:H	2.24	0.54
1:A:126:SER:O	1:A:148:VAL:HG13	2.08	0.54
1:B:504:VAL:CB	1:B:508:LYS:HD3	2.36	0.54
1:B:121:CYS:HB2	1:B:144:LYS:HG2	1.89	0.54
1:B:214:ILE:HG21	1:B:394:MET:HB2	1.90	0.54
1:B:435:ARG:NH2	1:B:457:LEU:HD23	2.23	0.54
1:B:479:PRO:CD	1:B:511:ARG:HG2	2.38	0.54
1:A:388:ILE:HD12	1:A:422:GLY:CA	2.38	0.53
1:C:108:GLU:OE1	1:C:135:LYS:HE3	2.08	0.53
1:B:479:PRO:HD2	1:B:511:ARG:CG	2.38	0.53
1:D:425:ASP:HB2	1:D:431:TYR:O	2.08	0.53
1:A:106:TYR:HE2	1:A:114:HIS:ND1	2.06	0.53
1:C:81:ASN:O	1:C:263:LYS:HD3	2.08	0.53
1:B:190:ALA:HB2	1:B:209:HIS:HD2	1.73	0.53
1:B:335:GLN:H	1:B:335:GLN:CD	2.12	0.53
1:C:342:THR:HG22	1:C:343:CYS:N	2.22	0.53
1:B:521:PRO:HG2	1:B:528:LEU:HA	1.91	0.53
1:C:253:PHE:HB2	1:C:254:PRO:HD3	1.91	0.53
1:A:333:ILE:O	1:A:334:LEU:HD13	2.09	0.53
1:B:449:PRO:HB2	1:B:453:GLU:HB3	1.90	0.53
1:C:222:PRO:O	1:C:227:ARG:HD3	2.09	0.53
1:A:372:ILE:O	1:A:380:LEU:CD1	2.56	0.53
1:A:382:PRO:CA	1:A:424:TYR:CD1	2.90	0.53
1:A:337:TYR:HE2	1:A:349:SER:HB2	1.74	0.53
1:C:286:PRO:O	1:C:289:MET:HB2	2.09	0.53
1:A:429:PHE:HB3	1:A:431:TYR:HE1	1.73	0.53
1:D:11:ARG:HG3	1:D:12:PRO:HD2	1.90	0.53
1:D:347:ILE:HD12	1:D:390:PHE:CZ	2.44	0.53
1:B:436:LEU:HD22	1:B:442:TYR:HD2	1.73	0.53
1:B:470:ILE:CD1	1:B:478:LEU:HB3	2.28	0.53
1:B:479:PRO:HD2	1:B:511:ARG:HG2	1.91	0.53
1:D:114:HIS:C	1:D:114:HIS:CD2	2.85	0.53
1:A:396:MET:HE3	1:A:416:LEU:HD11	1.90	0.52
1:D:342:THR:HG21	1:D:396:MET:N	2.24	0.52
1:A:347:ILE:CD1	1:A:390:PHE:CE1	2.92	0.52
1:D:149:ILE:HA	1:D:161:VAL:HG23	1.90	0.52
1:D:221:ASP:OD1	1:D:223:ILE:HG22	2.10	0.52
1:B:148:VAL:O	1:B:161:VAL:HG23	2.10	0.52
1:A:17:PHE:HZ	1:A:23:LEU:HD23	1.74	0.52
1:A:268:GLU:C	1:A:270:PHE:N	2.62	0.52
1:B:233:SER:HA	1:B:258:LYS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:TYR:HB2	1:B:448:ALA:O	2.10	0.52
1:C:114:HIS:C	1:C:114:HIS:CD2	2.88	0.52
1:D:90:ILE:HA	1:D:93:LEU:HD12	1.92	0.52
1:D:240:PHE:O	1:D:246:LEU:HB2	2.10	0.52
1:D:336:GLY:HA3	1:D:339:LEU:HD11	1.91	0.52
1:A:274:ILE:HG23	1:A:279:ILE:HB	1.91	0.52
1:B:470:ILE:HD12	1:B:478:LEU:CB	2.29	0.52
1:C:41:ASP:CG	1:C:44:THR:HG23	2.35	0.52
1:C:189:THR:HG23	1:C:206:VAL:HG13	1.92	0.52
1:D:421:LEU:HG	1:D:436:LEU:HB2	1.92	0.52
1:B:336:GLY:N	1:B:348:LEU:HB3	2.18	0.52
1:B:149:ILE:HA	1:B:161:VAL:CG2	2.40	0.51
1:C:335:GLN:NE2	1:C:336:GLY:N	2.57	0.51
1:B:456:LEU:O	1:B:456:LEU:HG	2.06	0.51
1:B:515:VAL:HB	1:B:537:PHE:CE1	2.44	0.51
1:C:380:LEU:HD12	1:C:384:GLU:OE2	2.11	0.51
1:D:286:PRO:O	1:D:289:MET:HB2	2.10	0.51
1:D:372:ILE:HG22	1:D:378:LYS:C	2.35	0.51
1:A:140:LEU:HB3	1:A:142:PHE:CZ	2.45	0.51
1:D:347:ILE:HA	1:D:363:PRO:N	2.25	0.51
1:B:11:ARG:CD	1:C:176:VAL:O	2.58	0.51
1:B:347:ILE:HG21	1:B:432:VAL:HG21	1.93	0.51
1:D:347:ILE:O	1:D:347:ILE:CG2	2.52	0.51
1:B:119:LYS:HG2	1:B:142:PHE:CD2	2.45	0.51
1:C:26:TYR:HB2	1:C:94:TYR:CE1	2.46	0.51
1:D:347:ILE:HG21	1:D:432:VAL:HG11	1.92	0.51
1:D:372:ILE:CG2	1:D:379:ALA:HA	2.41	0.51
1:C:130:LEU:HD21	1:C:158:VAL:HG21	1.91	0.51
1:D:13:ARG:NH1	1:D:13:ARG:CG	2.74	0.51
1:D:347:ILE:HG12	1:D:363:PRO:CA	2.36	0.51
1:A:149:ILE:HA	1:A:161:VAL:CG2	2.39	0.51
1:B:436:LEU:HD11	1:B:451:GLU:H	1.76	0.51
1:A:346:LEU:HD11	1:A:390:PHE:CD2	2.46	0.51
1:D:119:LYS:HA	1:D:142:PHE:CE2	2.46	0.51
1:D:422:GLY:HA2	1:D:435:ARG:H	1.75	0.51
1:A:223:ILE:HG22	1:A:224:TYR:CD1	2.46	0.51
1:A:284:VAL:HG22	1:A:289:MET:HE2	1.93	0.51
1:A:388:ILE:CD1	1:A:422:GLY:HA3	2.41	0.51
1:B:264:LYS:HD3	1:B:266:GLU:OE1	2.11	0.51
1:B:349:SER:O	1:B:349:SER:OG	2.29	0.51
1:B:472:ASP:O	1:B:478:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:SER:HA	1:C:114:HIS:CE1	2.46	0.51
1:C:112:ILE:HG23	1:C:140:LEU:HD21	1.93	0.51
1:A:370:LYS:O	1:A:388:ILE:HA	2.11	0.50
1:A:389:CYS:HB2	1:A:416:LEU:O	2.12	0.50
1:C:95:GLN:O	1:C:181:LYS:HE3	2.12	0.50
1:C:334:LEU:HB3	1:C:349:SER:HB3	1.93	0.50
1:B:264:LYS:HE2	1:B:265:PHE:CZ	2.47	0.50
1:B:455:LEU:CD2	1:B:467:VAL:HG22	2.42	0.50
1:B:472:ASP:O	1:B:478:LEU:CD1	2.51	0.50
1:A:17:PHE:CD2	1:A:24:GLN:HB2	2.47	0.50
1:B:234:ILE:HG13	1:B:235:LEU:N	2.27	0.50
1:B:318:ARG:HG2	1:B:319:ASP:OD1	2.12	0.50
1:A:311:CYS:HB3	1:A:335:GLN:HE21	1.75	0.50
1:B:482:CYS:HA	1:B:515:VAL:HG12	1.94	0.50
1:B:497:GLN:O	1:B:501:ALA:HB2	2.11	0.50
1:B:507:THR:HB	1:B:511:ARG:NH1	2.27	0.50
1:C:271:LEU:O	1:C:274:ILE:HG22	2.10	0.50
1:A:140:LEU:HB3	1:A:142:PHE:CE1	2.47	0.50
1:A:381:GLY:C	1:A:424:TYR:CD1	2.90	0.50
1:B:371:VAL:HG23	1:B:380:LEU:HB2	1.93	0.50
1:A:325:ALA:HB2	1:A:333:ILE:HG22	1.94	0.50
1:B:426:GLU:O	1:B:430:ILE:N	2.45	0.50
1:C:293:ALA:O	1:C:327:ARG:NH1	2.34	0.50
1:A:313:GLY:O	1:A:339:LEU:CD1	2.59	0.50
1:A:313:GLY:O	1:A:315:PRO:HD3	2.12	0.50
1:B:449:PRO:HB2	1:B:453:GLU:CB	2.40	0.50
1:A:334:LEU:HG	1:A:349:SER:OG	2.12	0.49
1:D:405:ALA:HA	1:D:408:ASP:HB3	1.92	0.49
1:A:125:CYS:SG	1:A:126:SER:N	2.85	0.49
1:B:283:VAL:HG22	1:B:310:ALA:HB3	1.92	0.49
1:B:309:ILE:HG12	1:B:330:VAL:HG21	1.93	0.49
1:D:86:PHE:HB3	1:D:90:ILE:HD12	1.94	0.49
1:D:347:ILE:HD11	1:D:390:PHE:CE1	2.47	0.49
1:B:446:GLN:O	1:B:447:VAL:O	2.30	0.49
1:D:13:ARG:NH1	1:D:221:ASP:CG	2.61	0.49
1:D:388:ILE:O	1:D:418:THR:HB	2.13	0.49
1:A:27:GLN:CG	1:D:15:LEU:HD12	2.43	0.49
1:A:334:LEU:O	1:A:335:GLN:CB	2.60	0.49
1:A:288:ILE:O	1:A:292:LEU:HG	2.12	0.49
1:B:297:LEU:HB3	1:B:300:GLU:HG3	1.95	0.49
1:D:264:LYS:HD3	1:D:266:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:THR:OG1	1:A:396:MET:HE2	2.12	0.49
1:B:531:ASN:H	1:B:531:ASN:ND2	2.11	0.49
1:C:373:ASP:HB3	1:C:377:GLY:H	1.77	0.49
1:D:107:THR:HG23	1:D:109:ARG:HB3	1.94	0.49
1:D:268:GLU:C	1:D:270:PHE:N	2.65	0.49
1:A:286:PRO:HA	1:A:289:MET:HB2	1.94	0.49
1:A:364:MET:O	1:A:367:VAL:HB	2.11	0.49
1:B:159:GLU:OE1	1:B:167:ARG:NH1	2.42	0.49
1:B:462:ILE:O	1:B:462:ILE:HG13	2.10	0.49
1:A:14:ASP:OD2	1:D:31:LYS:HE3	2.12	0.49
1:A:61:ALA:HB1	1:A:95:GLN:HE21	1.78	0.49
1:B:367:VAL:HA	1:B:392:SER:HB2	1.94	0.49
1:C:382:PRO:HA	1:C:424:TYR:CB	2.43	0.49
1:C:402:ASN:O	1:C:406:THR:HG23	2.12	0.49
1:D:13:ARG:HG3	1:D:13:ARG:HH11	1.78	0.49
1:D:372:ILE:HA	1:D:379:ALA:HA	1.94	0.49
1:B:455:LEU:HD21	1:B:466:GLY:N	2.28	0.48
1:D:289:MET:HE1	1:D:309:ILE:HG22	1.95	0.48
1:A:306:LEU:HG	1:A:309:ILE:HD11	1.95	0.48
1:B:8:ASN:O	1:B:367:VAL:O	2.30	0.48
1:B:11:ARG:HD3	1:C:176:VAL:O	2.13	0.48
1:B:234:ILE:HD12	1:B:281:SER:HB3	1.95	0.48
1:B:274:ILE:HG13	1:B:279:ILE:HB	1.96	0.48
1:D:294:LYS:HD3	1:D:323:LYS:HE3	1.94	0.48
1:D:347:ILE:CG2	1:D:432:VAL:CG2	2.90	0.48
1:D:380:LEU:HD12	1:D:384:GLU:CD	2.37	0.48
1:B:426:GLU:HB3	1:B:429:PHE:HD2	1.76	0.48
1:C:292:LEU:HB3	1:C:324:VAL:HG11	1.94	0.48
1:B:435:ARG:NH2	1:B:457:LEU:CD2	2.76	0.48
1:D:338:GLY:O	1:D:339:LEU:C	2.56	0.48
1:B:77:ILE:HG22	1:B:99:MET:SD	2.54	0.48
1:A:374:ILE:H	1:A:374:ILE:HG13	1.49	0.48
1:B:478:LEU:HG	1:B:511:ARG:CB	2.40	0.48
1:A:388:ILE:HD12	1:A:422:GLY:HA3	1.96	0.48
1:C:297:LEU:HB3	1:C:300:GLU:CD	2.38	0.48
1:D:13:ARG:HH11	1:D:13:ARG:CG	2.25	0.48
1:D:190:ALA:HB2	1:D:209:HIS:CD2	2.48	0.48
1:D:211:SER:HA	1:D:394:MET:HA	1.96	0.48
1:A:382:PRO:CA	1:A:424:TYR:HD1	2.16	0.48
1:B:199:THR:OG1	1:B:203:LYS:NZ	2.45	0.48
1:B:342:THR:HB	1:B:343:CYS:H	1.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:GLY:HA3	1:C:341:GLU:OE1	2.14	0.48
1:A:240:PHE:O	1:A:246:LEU:HB2	2.14	0.48
1:C:235:LEU:HD21	1:C:237:ILE:HB	1.96	0.48
1:D:271:LEU:H	1:D:271:LEU:HD22	1.79	0.48
1:B:9:GLY:HA2	1:B:363:PRO:HB2	1.95	0.47
1:D:396:MET:C	1:D:398:GLY:H	2.22	0.47
1:A:27:GLN:CD	1:D:15:LEU:HD11	2.39	0.47
1:A:176:VAL:O	1:D:11:ARG:NH1	2.47	0.47
1:C:185:PRO:HG2	1:C:210:ARG:NH2	2.29	0.47
1:B:114:HIS:CD2	1:B:114:HIS:C	2.91	0.47
1:B:336:GLY:N	1:B:348:LEU:CB	2.75	0.47
1:B:335:GLN:N	1:B:335:GLN:CD	2.73	0.47
1:D:315:PRO:HG3	1:D:335:GLN:HE22	1.80	0.47
1:A:89:LEU:HA	1:A:99:MET:HE3	1.96	0.47
1:A:224:TYR:CD2	1:A:364:MET:HE3	2.49	0.47
1:A:234:ILE:HG13	1:A:235:LEU:N	2.29	0.47
1:B:137:GLN:HG2	1:B:137:GLN:O	2.15	0.47
1:B:496:VAL:CB	1:B:514:VAL:HG21	2.39	0.47
1:A:236:ALA:HB2	1:A:252:TYR:CE2	2.44	0.47
1:C:372:ILE:HD11	1:C:387:GLU:HB3	1.96	0.47
1:D:36:THR:HA	1:D:49:SER:HB2	1.97	0.47
1:D:230:PRO:O	1:D:231:ASP:HB2	2.15	0.47
1:D:251:ALA:O	1:D:254:PRO:HD2	2.14	0.47
1:A:337:TYR:HD2	1:A:348:LEU:C	2.22	0.47
1:B:106:TYR:HB2	1:B:111:MET:HE2	1.97	0.47
1:A:388:ILE:HD12	1:A:422:GLY:N	2.30	0.47
1:B:119:LYS:HA	1:B:142:PHE:CE2	2.50	0.47
1:D:371:VAL:HG13	1:D:371:VAL:O	2.15	0.47
1:D:422:GLY:CA	1:D:435:ARG:H	2.28	0.47
1:A:63:SER:OG	1:A:165:VAL:HA	2.15	0.47
1:B:83:ILE:HD13	1:B:261:MET:HE1	1.97	0.47
1:A:399:TYR:N	1:A:399:TYR:CD1	2.83	0.46
1:C:284:VAL:O	1:C:311:CYS:HA	2.16	0.46
1:D:28:SER:OG	1:D:254:PRO:HA	2.15	0.46
1:D:334:LEU:HB3	1:D:349:SER:HB3	1.96	0.46
1:A:159:GLU:OE1	1:A:167:ARG:NH1	2.49	0.46
1:A:342:THR:CG2	1:A:343:CYS:H	2.23	0.46
1:B:506:THR:O	1:B:507:THR:HG23	2.15	0.46
1:C:211:SER:HA	1:C:394:MET:HA	1.96	0.46
1:C:214:ILE:O	1:C:217:VAL:HB	2.16	0.46
1:D:152:MET:HE1	1:D:162:PHE:CD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:LYS:HD3	1:D:399:TYR:HE2	1.80	0.46
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.81	0.46
1:C:382:PRO:HA	1:C:424:TYR:CG	2.50	0.46
1:B:147:ILE:HA	1:B:159:GLU:O	2.14	0.46
1:B:481:ALA:CB	1:B:510:LEU:HD22	2.45	0.46
1:C:318:ARG:HA	1:C:319:ASP:HA	1.60	0.46
1:B:13:ARG:NH1	1:B:221:ASP:OD2	2.48	0.46
1:A:230:PRO:HB3	1:A:255:VAL:O	2.15	0.46
1:B:84:HIS:O	1:B:88:PRO:HD2	2.16	0.46
1:B:271:LEU:CD1	1:B:303:LEU:HD11	2.46	0.46
1:B:288:ILE:O	1:B:292:LEU:HB2	2.15	0.46
1:C:385:LYS:HA	1:C:422:GLY:O	2.15	0.46
1:C:399:TYR:N	1:C:399:TYR:CD1	2.84	0.46
1:D:293:ALA:HB2	1:D:324:VAL:HG13	1.97	0.46
1:B:8:ASN:O	1:B:368:GLN:HA	2.15	0.46
1:B:91:ALA:HA	1:B:94:TYR:CD2	2.51	0.46
1:B:337:TYR:C	1:B:337:TYR:CD2	2.93	0.46
1:B:446:GLN:O	1:B:446:GLN:HG3	2.16	0.46
1:C:213:THR:O	1:C:217:VAL:HG23	2.15	0.46
1:A:372:ILE:O	1:A:373:ASP:HB2	2.16	0.46
1:D:112:ILE:HG23	1:D:140:LEU:HD21	1.97	0.46
1:D:303:LEU:C	1:D:305:SER:H	2.23	0.46
1:B:274:ILE:HG23	1:B:303:LEU:HD22	1.97	0.46
1:C:364:MET:CG	1:C:365:PRO:HD3	2.29	0.46
1:A:253:PHE:HB2	1:A:254:PRO:HD3	1.97	0.46
1:B:17:PHE:O	1:B:213:THR:HG21	2.16	0.46
1:B:306:LEU:HD12	1:B:306:LEU:HA	1.71	0.46
1:B:373:ASP:HB2	1:B:377:GLY:N	2.31	0.46
1:B:492:THR:O	1:B:496:VAL:HG23	2.15	0.46
1:C:96:GLY:HA3	1:C:188:ARG:NH1	2.31	0.46
1:C:108:GLU:CD	1:C:135:LYS:HE3	2.41	0.46
1:A:152:MET:HE1	1:A:162:PHE:CG	2.51	0.45
1:A:318:ARG:O	1:A:318:ARG:HG3	2.16	0.45
1:B:319:ASP:OD1	1:B:319:ASP:N	2.49	0.45
1:B:484:VAL:HG11	1:B:519:SER:O	2.16	0.45
1:A:90:ILE:HA	1:A:93:LEU:HD12	1.98	0.45
1:B:519:SER:OG	1:B:520:ILE:N	2.37	0.45
1:C:389:CYS:HB3	1:C:417:HIS:HA	1.97	0.45
1:A:16:VAL:HA	1:A:217:VAL:CG2	2.47	0.45
1:A:190:ALA:HB2	1:A:209:HIS:CD2	2.51	0.45
1:A:347:ILE:C	1:A:348:LEU:HD12	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:GLY:O	1:B:315:PRO:HD3	2.17	0.45
1:C:231:ASP:OD1	1:C:258:LYS:HE2	2.16	0.45
1:C:286:PRO:HG2	1:C:287:PRO:HD3	1.97	0.45
1:C:371:VAL:HG21	1:C:384:GLU:O	2.16	0.45
1:D:210:ARG:NH1	1:D:393:GLN:OE1	2.49	0.45
1:A:269:PHE:HA	1:A:272:LYS:HB3	1.98	0.45
1:A:423:TYR:C	1:A:424:TYR:O	2.59	0.45
1:C:159:GLU:HG2	1:C:163:SER:HB2	1.97	0.45
1:C:346:LEU:HD12	1:C:346:LEU:O	2.16	0.45
1:D:16:VAL:HG13	1:D:16:VAL:O	2.15	0.45
1:A:84:HIS:HB2	1:A:149:ILE:HD12	1.98	0.45
1:B:78:CYS:HB3	1:B:133:ILE:HD11	1.99	0.45
1:B:205:VAL:CG1	1:B:342:THR:HG23	2.46	0.45
1:B:319:ASP:O	1:B:323:LYS:HG3	2.16	0.45
1:C:291:TYR:O	1:C:295:SER:HB3	2.16	0.45
1:A:71:HIS:CD2	1:A:71:HIS:H	2.33	0.45
1:A:370:LYS:HG2	1:A:415:TRP:CZ3	2.52	0.45
1:A:372:ILE:HD12	1:A:373:ASP:O	2.16	0.45
1:B:280:ALA:O	1:B:306:LEU:HD12	2.17	0.45
1:C:83:ILE:H	1:C:83:ILE:HG12	1.52	0.45
1:A:296:PRO:O	1:A:298:VAL:HG13	2.17	0.45
1:B:289:MET:HE3	1:B:311:CYS:HB2	1.99	0.45
1:B:307:THR:HG22	1:B:308:GLU:HG3	1.99	0.45
1:B:511:ARG:HA	1:B:511:ARG:HD3	1.37	0.45
1:D:372:ILE:C	1:D:380:LEU:HD23	2.31	0.45
1:A:74:VAL:HG12	1:A:120:PRO:HB3	1.98	0.45
1:B:102:SER:HA	1:B:114:HIS:HE1	1.81	0.45
1:B:454:ASN:OD1	1:B:455:LEU:N	2.50	0.45
1:C:139:HIS:O	1:C:140:LEU:HD23	2.16	0.45
1:C:296:PRO:HB2	1:C:297:LEU:HG	1.99	0.45
1:D:9:GLY:HA2	1:D:363:PRO:CG	2.47	0.45
1:A:399:TYR:N	1:A:399:TYR:HD1	2.15	0.45
1:B:402:ASN:O	1:B:406:THR:HG23	2.17	0.45
1:C:59:ARG:NH2	1:C:170:ASP:O	2.50	0.45
1:A:268:GLU:HB2	1:A:269:PHE:H	1.38	0.44
1:B:439:LEU:HA	1:B:442:TYR:CE2	2.52	0.44
1:B:501:ALA:HA	1:B:509:HIS:CD2	2.52	0.44
1:B:510:LEU:HD22	1:B:514:VAL:HG22	1.98	0.44
1:C:372:ILE:HB	1:C:373:ASP:H	1.60	0.44
1:D:75:VAL:HG12	1:D:122:LEU:HB3	1.98	0.44
1:D:303:LEU:HD12	1:D:328:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD21	1:A:291:TYR:HE2	1.81	0.44
1:C:396:MET:C	1:C:398:GLY:H	2.25	0.44
1:D:286:PRO:HD3	1:D:311:CYS:SG	2.57	0.44
1:A:107:THR:HG23	1:A:109:ARG:HB3	2.00	0.44
1:A:284:VAL:HB	1:A:288:ILE:HG13	1.99	0.44
1:B:251:ALA:O	1:B:254:PRO:HD2	2.17	0.44
1:B:435:ARG:HH22	1:B:457:LEU:HD23	1.79	0.44
1:D:49:SER:N	1:D:52:GLN:OE1	2.42	0.44
1:D:323:LYS:O	1:D:327:ARG:HG3	2.17	0.44
1:A:286:PRO:HG2	1:A:287:PRO:HD3	1.98	0.44
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.86	0.44
1:B:207:ILE:HD13	1:B:342:THR:HG22	1.99	0.44
1:B:215:ARG:NH2	1:B:248:THR:HG22	2.32	0.44
1:D:13:ARG:HG3	1:D:221:ASP:CG	2.42	0.44
1:D:228:ILE:HG12	1:D:229:ALA:N	2.32	0.44
1:A:152:MET:HE1	1:A:162:PHE:CD1	2.53	0.44
1:A:210:ARG:O	1:A:214:ILE:HG13	2.18	0.44
1:B:215:ARG:HH21	1:B:248:THR:HG22	1.82	0.44
1:D:402:ASN:O	1:D:406:THR:HG23	2.18	0.44
1:A:422:GLY:CA	1:A:434:ASP:HA	2.48	0.44
1:B:336:GLY:HA3	1:B:348:LEU:HD23	1.99	0.44
1:B:454:ASN:O	1:B:456:LEU:N	2.51	0.44
1:B:457:LEU:HD13	1:B:457:LEU:HA	1.75	0.44
1:A:102:SER:HA	1:A:114:HIS:HE1	1.83	0.44
1:A:218:HIS:HB3	1:A:364:MET:HE1	2.00	0.44
1:A:382:PRO:HB3	1:A:426:GLU:HA	2.00	0.44
1:A:18:PRO:O	1:A:185:PRO:HG3	2.17	0.44
1:B:102:SER:HA	1:B:114:HIS:CE1	2.52	0.44
1:D:9:GLY:HA2	1:D:363:PRO:HG2	2.00	0.44
1:B:211:SER:O	1:B:215:ARG:HB2	2.18	0.44
1:B:441:LYS:HE2	1:B:530:ARG:CB	2.41	0.44
1:C:36:THR:HA	1:C:49:SER:HB2	1.99	0.44
1:A:15:LEU:HA	1:A:15:LEU:HD23	1.80	0.43
1:A:41:ASP:HB3	1:A:44:THR:HG23	2.00	0.43
1:A:326:LYS:NZ	1:A:326:LYS:HA	2.32	0.43
1:A:398:GLY:C	1:A:399:TYR:HD1	2.26	0.43
1:C:399:TYR:N	1:C:399:TYR:HD1	2.15	0.43
1:B:13:ARG:HG3	1:B:13:ARG:HH11	1.83	0.43
1:C:7:VAL:HB	1:C:369:VAL:HG13	2.00	0.43
1:C:364:MET:HG2	1:C:365:PRO:N	2.29	0.43
1:B:16:VAL:HA	1:B:217:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HA	1:B:134:LEU:HD23	1.73	0.43
1:B:493:GLU:HG3	1:B:513:GLY:CA	2.49	0.43
1:D:79:SER:OG	1:D:126:SER:HB2	2.18	0.43
1:B:509:HIS:C	1:B:510:LEU:HG	2.43	0.43
1:D:186:LEU:HD23	1:D:186:LEU:O	2.18	0.43
1:A:348:LEU:N	1:A:348:LEU:CD1	2.82	0.43
1:B:103:ASN:HD22	1:B:241:HIS:CE1	2.37	0.43
1:C:234:ILE:HG13	1:C:235:LEU:N	2.32	0.43
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.71	0.43
1:C:274:ILE:HD11	1:C:306:LEU:CD2	2.48	0.43
1:C:315:PRO:CB	1:C:335:GLN:HE22	2.31	0.43
1:C:337:TYR:O	1:C:347:ILE:HG12	2.18	0.43
1:D:313:GLY:O	1:D:315:PRO:HD3	2.18	0.43
1:A:378:LYS:HB3	1:A:379:ALA:H	1.69	0.43
1:C:288:ILE:O	1:C:292:LEU:HB2	2.19	0.43
1:D:372:ILE:HD12	1:D:373:ASP:N	2.33	0.43
1:C:8:ASN:HA	1:C:368:GLN:HG2	1.99	0.43
1:A:311:CYS:H	1:A:335:GLN:CB	2.31	0.43
1:A:346:LEU:HD11	1:A:390:PHE:CE2	2.54	0.43
1:B:125:CYS:SG	1:B:126:SER:N	2.92	0.43
1:C:198:THR:HG22	1:C:199:THR:HG23	2.01	0.43
1:D:382:PRO:HA	1:D:424:TYR:HB3	1.99	0.43
1:D:425:ASP:CG	1:D:433:VAL:HG22	2.44	0.43
1:A:337:TYR:CD2	1:A:348:LEU:C	2.97	0.42
1:B:41:ASP:OD1	1:B:43:HIS:HB2	2.19	0.42
1:B:296:PRO:O	1:B:298:VAL:HG13	2.19	0.42
1:B:308:GLU:C	1:B:309:ILE:HG12	2.44	0.42
1:B:330:VAL:O	1:B:332:GLY:N	2.52	0.42
1:B:336:GLY:HA3	1:B:348:LEU:CB	2.26	0.42
1:B:481:ALA:HB2	1:B:510:LEU:HD22	2.00	0.42
1:D:284:VAL:HG21	1:D:288:ILE:HG22	2.01	0.42
1:D:339:LEU:HD12	1:D:339:LEU:H	1.84	0.42
1:B:24:GLN:OE1	1:B:216:PHE:HD2	2.01	0.42
1:C:234:ILE:HD12	1:C:281:SER:HB3	2.01	0.42
1:B:335:GLN:O	1:B:348:LEU:CB	2.58	0.42
1:C:289:MET:HE1	1:C:333:ILE:HD12	2.02	0.42
1:C:328:LEU:O	1:C:329:LYS:C	2.62	0.42
1:A:201:LEU:HD12	1:A:202:PRO:HD2	2.02	0.42
1:B:330:VAL:C	1:B:332:GLY:H	2.27	0.42
1:B:491:MET:HE2	1:B:496:VAL:HG22	2.00	0.42
1:B:517:ILE:HD13	1:B:540:GLU:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ILE:HB	1:C:83:ILE:HG23	2.00	0.42
1:C:274:ILE:HD12	1:C:282:ILE:HG21	2.01	0.42
1:D:286:PRO:HA	1:D:289:MET:HB2	2.00	0.42
1:D:289:MET:HE3	1:D:311:CYS:HB2	2.01	0.42
1:D:309:ILE:HB	1:D:333:ILE:HD12	2.00	0.42
1:A:203:LYS:HD2	1:A:399:TYR:CD2	2.55	0.42
1:B:41:ASP:CG	1:B:44:THR:HG23	2.45	0.42
1:B:107:THR:HG22	1:B:110:GLU:HG3	2.01	0.42
1:B:328:LEU:HA	1:B:328:LEU:HD23	1.50	0.42
1:C:224:TYR:CG	1:C:364:MET:HE2	2.54	0.42
1:B:9:GLY:CA	1:B:363:PRO:HB2	2.49	0.42
1:B:111:MET:HE3	1:B:132:PHE:HE2	1.83	0.42
1:B:436:LEU:HD22	1:B:442:TYR:CD2	2.51	0.42
1:D:268:GLU:HG2	1:D:269:PHE:N	2.35	0.42
1:A:32:TYR:HB3	1:A:35:ILE:HD12	2.01	0.42
1:A:179:ASN:HA	1:A:180:PRO:HD3	1.91	0.42
1:B:229:ALA:HA	1:B:230:PRO:HD2	1.76	0.42
1:D:159:GLU:CD	1:D:167:ARG:HH11	2.27	0.42
1:A:271:LEU:HB3	1:A:301:TYR:CD1	2.55	0.42
1:B:215:ARG:HD2	1:B:215:ARG:HA	1.78	0.42
1:B:322:ASP:OD1	1:B:322:ASP:N	2.52	0.42
1:B:470:ILE:H	1:B:470:ILE:HG13	1.52	0.42
1:C:71:HIS:CD2	1:C:71:HIS:H	2.36	0.42
1:C:309:ILE:HG12	1:C:330:VAL:HG21	2.02	0.42
1:A:107:THR:HG23	1:A:110:GLU:H	1.84	0.42
1:A:395:LEU:HA	1:A:395:LEU:HD23	1.90	0.42
1:B:101:THR:HG21	1:B:246:LEU:CD1	2.50	0.42
1:B:326:LYS:HA	1:B:326:LYS:HD2	1.69	0.42
1:B:485:LEU:HD13	1:B:489:LYS:O	2.20	0.42
1:C:185:PRO:O	1:C:210:ARG:N	2.48	0.42
1:C:330:VAL:O	1:C:332:GLY:N	2.44	0.42
1:D:317:GLY:C	1:D:319:ASP:H	2.28	0.42
1:A:59:ARG:HB3	1:A:165:VAL:CG1	2.50	0.41
1:A:127:LYS:HB2	1:A:150:ASP:OD1	2.19	0.41
1:A:203:LYS:HD2	1:A:399:TYR:CE2	2.55	0.41
1:A:233:SER:HA	1:A:258:LYS:O	2.19	0.41
1:A:389:CYS:HB3	1:A:417:HIS:HA	2.01	0.41
1:B:479:PRO:HG2	1:B:480:SER:H	1.85	0.41
1:C:335:GLN:HB2	1:C:336:GLY:H	1.66	0.41
1:C:423:TYR:HD2	1:C:424:TYR:O	2.03	0.41
1:A:347:ILE:HD12	1:A:390:PHE:HE1	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ARG:HD3	1:C:176:VAL:HG12	2.01	0.41
1:B:82:ASN:O	1:B:84:HIS:N	2.52	0.41
1:B:183:PHE:CE2	1:B:188:ARG:HG2	2.55	0.41
1:B:439:LEU:HA	1:B:442:TYR:HE2	1.85	0.41
1:B:460:PRO:HA	1:B:461:ASN:HA	1.75	0.41
1:B:466:GLY:HA3	1:B:482:CYS:H	1.85	0.41
1:C:347:ILE:HG13	1:C:432:VAL:CG2	2.50	0.41
1:D:271:LEU:O	1:D:274:ILE:HG22	2.20	0.41
1:D:348:LEU:HB2	1:D:349:SER:H	1.68	0.41
1:A:339:LEU:O	1:A:340:THR:CG2	2.66	0.41
1:B:198:THR:O	1:B:200:GLY:N	2.49	0.41
1:B:284:VAL:HB	1:B:288:ILE:HD11	2.02	0.41
1:A:287:PRO:O	1:A:290:VAL:HG22	2.20	0.41
1:A:381:GLY:C	1:A:424:TYR:CE1	2.98	0.41
1:C:372:ILE:O	1:C:386:GLY:HA3	2.21	0.41
1:D:382:PRO:HA	1:D:424:TYR:CB	2.51	0.41
1:A:41:ASP:HB2	1:A:83:ILE:HD11	2.01	0.41
1:A:112:ILE:HG23	1:A:140:LEU:CD2	2.51	0.41
1:A:385:LYS:HB3	1:A:421:LEU:HD13	2.01	0.41
1:B:453:GLU:O	1:B:457:LEU:HD23	2.20	0.41
1:D:134:LEU:HD23	1:D:134:LEU:HA	1.85	0.41
1:A:431:TYR:HE2	1:A:433:VAL:HG23	1.86	0.41
1:B:236:ALA:O	1:B:261:MET:HA	2.21	0.41
1:B:473:GLU:H	1:B:478:LEU:HD13	1.85	0.41
1:B:497:GLN:CG	1:B:510:LEU:HD11	2.29	0.41
1:C:20:THR:HG23	1:C:23:LEU:CB	2.50	0.41
1:C:315:PRO:CG	1:C:336:GLY:HA3	2.51	0.41
1:A:41:ASP:CG	1:A:44:THR:HG23	2.45	0.41
1:A:328:LEU:O	1:A:329:LYS:C	2.63	0.41
1:A:383:ARG:HA	1:A:423:TYR:CD2	2.48	0.41
1:B:383:ARG:HA	1:B:423:TYR:HD2	1.80	0.41
1:C:149:ILE:HA	1:C:161:VAL:HG23	2.01	0.41
1:C:339:LEU:CD2	1:C:344:SER:OG	2.66	0.41
1:D:59:ARG:HH12	1:D:173:PHE:HB3	1.84	0.41
1:D:69:LEU:HA	1:D:69:LEU:HD23	1.82	0.41
1:D:186:LEU:HD11	1:D:393:GLN:HG2	2.03	0.41
1:D:199:THR:OG1	1:D:200:GLY:N	2.51	0.41
1:A:36:THR:HA	1:A:49:SER:HB2	2.03	0.41
1:A:178:PHE:CD1	1:A:178:PHE:C	2.98	0.41
1:A:370:LYS:HE2	1:A:415:TRP:CD2	2.56	0.41
1:B:81:ASN:HB2	1:B:263:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LEU:HD21	1:B:237:ILE:HB	2.03	0.41
1:B:339:LEU:C	1:B:341:GLU:H	2.29	0.41
1:B:420:ASP:N	1:B:420:ASP:OD1	2.54	0.41
1:B:486:GLU:HB2	1:B:487:PRO:HD3	2.02	0.41
1:C:149:ILE:HA	1:C:161:VAL:CG2	2.50	0.41
1:C:179:ASN:HA	1:C:180:PRO:HD3	1.89	0.41
1:C:190:ALA:HB2	1:C:209:HIS:CD2	2.56	0.41
1:D:61:ALA:HB1	1:D:95:GLN:NE2	2.36	0.41
1:D:83:ILE:H	1:D:83:ILE:HG12	1.64	0.41
1:D:120:PRO:HD2	1:D:142:PHE:HE2	1.85	0.41
1:D:271:LEU:HA	1:D:274:ILE:HG22	2.02	0.41
1:D:347:ILE:HA	1:D:363:PRO:HA	2.01	0.41
1:D:425:ASP:OD1	1:D:433:VAL:HG22	2.20	0.41
1:A:330:VAL:O	1:A:332:GLY:N	2.47	0.41
1:B:473:GLU:C	1:B:475:ALA:N	2.78	0.41
1:C:122:LEU:HD12	1:C:145:LYS:O	2.21	0.41
1:D:296:PRO:O	1:D:298:VAL:HG13	2.21	0.41
1:D:395:LEU:HA	1:D:395:LEU:HD23	1.79	0.41
1:A:185:PRO:O	1:A:210:ARG:N	2.52	0.40
1:A:196:SER:O	1:A:200:GLY:HA2	2.21	0.40
1:A:284:VAL:HB	1:A:288:ILE:CD1	2.51	0.40
1:B:388:ILE:HG22	1:B:418:THR:HG21	2.02	0.40
1:B:455:LEU:HD23	1:B:467:VAL:CG2	2.50	0.40
1:B:493:GLU:HG3	1:B:514:VAL:N	2.37	0.40
1:D:145:LYS:HE2	1:D:159:GLU:OE1	2.20	0.40
1:D:268:GLU:HA	1:D:271:LEU:HD23	2.03	0.40
1:A:346:LEU:HD12	1:A:347:ILE:HG13	2.03	0.40
1:B:270:PHE:O	1:B:274:ILE:HG22	2.20	0.40
1:B:345:ALA:C	1:B:346:LEU:HD12	2.46	0.40
1:A:422:GLY:HA2	1:A:434:ASP:HA	2.03	0.40
1:B:58:CYS:O	1:B:62:VAL:HG23	2.21	0.40
1:B:71:HIS:HB3	1:B:188:ARG:NH1	2.36	0.40
1:B:335:GLN:OE1	1:B:335:GLN:CA	2.70	0.40
1:B:347:ILE:CG1	1:B:363:PRO:HA	2.50	0.40
1:B:380:LEU:HB3	1:B:381:GLY:H	1.60	0.40
1:B:479:PRO:O	1:B:480:SER:HB3	2.21	0.40
1:D:76:ALA:HA	1:D:100:ALA:O	2.21	0.40
1:A:306:LEU:HD12	1:A:306:LEU:HA	1.87	0.40
1:A:372:ILE:C	1:A:380:LEU:HD13	2.46	0.40
1:C:103:ASN:ND2	1:C:241:HIS:CE1	2.85	0.40
1:C:282:ILE:HD12	1:C:284:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:PRO:O	1:D:185:PRO:HG3	2.20	0.40
1:D:123:MET:HE3	1:D:133:ILE:HD12	2.04	0.40
1:B:372:ILE:O	1:B:386:GLY:HA3	2.21	0.40
1:C:20:THR:HG23	1:C:23:LEU:HB2	2.02	0.40
1:C:223:ILE:HG22	1:C:224:TYR:CD1	2.56	0.40
1:C:255:VAL:HG23	1:C:257:LEU:HG	2.02	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	415/546 (76%)	342 (82%)	54 (13%)	19 (5%)	2	17
1	B	524/546 (96%)	397 (76%)	88 (17%)	39 (7%)	1	9
1	C	413/546 (76%)	355 (86%)	43 (10%)	15 (4%)	2	22
1	D	412/546 (76%)	343 (83%)	54 (13%)	15 (4%)	2	22
All	All	1764/2184 (81%)	1437 (82%)	239 (14%)	88 (5%)	1	16

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	231	ASP
1	A	319	ASP
1	A	378	LYS
1	A	379	ALA
1	A	401	ASN
1	A	430	ILE
1	B	83	ILE
1	B	344	SER

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Mol	Chain	Res	Type
1	B	347	ILE
1	B	430	ILE
1	B	437	LYS
1	B	446	GLN
1	B	447	VAL
1	B	460	PRO
1	B	479	PRO
1	B	530	ARG
1	C	198	THR
1	C	231	ASP
1	C	317	GLY
1	C	372	ILE
1	C	430	ILE
1	D	203	LYS
1	D	231	ASP
1	D	268	GLU
1	D	336	GLY
1	D	339	LEU
1	D	347	ILE
1	D	430	ILE
1	A	71	HIS
1	A	265	PHE
1	A	267	GLY
1	A	268	GLU
1	A	332	GLY
1	A	335	GLN
1	A	347	ILE
1	A	372	ILE
1	A	373	ASP
1	B	5	ASN
1	B	199	THR
1	B	319	ASP
1	B	442	TYR
1	B	465	ALA
1	B	514	VAL
1	B	522	LYS
1	B	543	LYS
1	C	8	ASN
1	C	71	HIS
1	C	332	GLY
1	D	71	HIS
1	D	332	GLY

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Mol	Chain	Res	Type
1	B	231	ASP
1	B	342	THR
1	B	400	HIS
1	B	467	VAL
1	B	525	THR
1	C	335	GLN
1	C	336	GLY
1	D	269	PHE
1	D	372	ILE
1	A	331	HIS
1	A	424	TYR
1	B	45	ASN
1	B	425	ASP
1	B	511	ARG
1	B	520	ILE
1	B	538	ALA
1	C	331	HIS
1	C	400	HIS
1	D	318	ARG
1	A	269	PHE
1	B	8	ASN
1	B	55	GLU
1	B	318	ARG
1	B	345	ALA
1	B	458	GLN
1	B	486	GLU
1	B	521	PRO
1	B	523	GLY
1	D	10	ASP
1	B	376	THR
1	B	528	LEU
1	C	347	ILE
1	D	200	GLY
1	D	230	PRO
1	B	237	ILE
1	C	225	GLY
1	C	230	PRO

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	365/471 (78%)	329 (90%)	36 (10%)	7	31
1	B	456/471 (97%)	385 (84%)	71 (16%)	2	16
1	C	363/471 (77%)	336 (93%)	27 (7%)	13	39
1	D	362/471 (77%)	335 (92%)	27 (8%)	12	39
All	All	1546/1884 (82%)	1385 (90%)	161 (10%)	7	29

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	27	GLN
1	A	44	THR
1	A	56	THR
1	A	62	VAL
1	A	118	SER
1	A	128	LYS
1	A	140	LEU
1	A	163	SER
1	A	165	VAL
1	A	196	SER
1	A	223	ILE
1	A	234	ILE
1	A	260	VAL
1	A	268	GLU
1	A	284	VAL
1	A	288	ILE
1	A	294	LYS
1	A	306	LEU
1	A	309	ILE
1	A	316	LEU
1	A	318	ARG
1	A	326	LYS
1	A	334	LEU
1	A	335	GLN
1	A	339	LEU
1	A	343	CYS
1	A	374	ILE

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Mol	Chain	Res	Type
1	A	378	LYS
1	A	380	LEU
1	A	383	ARG
1	A	388	ILE
1	A	412	LYS
1	A	418	THR
1	A	428	ARG
1	A	437	LYS
1	B	6	ILE
1	B	7	VAL
1	B	11	ARG
1	B	20	THR
1	B	36	THR
1	B	60	LEU
1	B	62	VAL
1	B	77	ILE
1	B	93	LEU
1	B	118	SER
1	B	119	LYS
1	B	126	SER
1	B	163	SER
1	B	165	VAL
1	B	182	GLU
1	B	187	GLU
1	B	193	MET
1	B	196	SER
1	B	223	ILE
1	B	228	ILE
1	B	234	ILE
1	B	260	VAL
1	B	266	GLU
1	B	288	ILE
1	B	292	LEU
1	B	294	LYS
1	B	309	ILE
1	B	316	LEU
1	B	320	ILE
1	B	326	LYS
1	B	329	LYS
1	B	335	GLN
1	B	337	TYR
1	B	342	THR

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Mol	Chain	Res	Type
1	B	343	CYS
1	B	346	LEU
1	B	368	GLN
1	B	369	VAL
1	B	378	LYS
1	B	388	ILE
1	B	389	CYS
1	B	420	ASP
1	B	421	LEU
1	B	428	ARG
1	B	433	VAL
1	B	436	LEU
1	B	439	LEU
1	B	445	TYR
1	B	451	GLU
1	B	452	LEU
1	B	455	LEU
1	B	456	LEU
1	B	457	LEU
1	B	459	HIS
1	B	462	ILE
1	B	467	VAL
1	B	468	ILE
1	B	470	ILE
1	B	472	ASP
1	B	477	GLN
1	B	484	VAL
1	B	485	LEU
1	B	492	THR
1	B	506	THR
1	B	508	LYS
1	B	510	LEU
1	B	511	ARG
1	B	515	VAL
1	B	531	ASN
1	B	532	GLU
1	B	543	LYS
1	C	20	THR
1	C	27	GLN
1	C	36	THR
1	C	44	THR
1	C	47	VAL

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Mol	Chain	Res	Type
1	C	56	THR
1	C	118	SER
1	C	155	ILE
1	C	165	VAL
1	C	223	ILE
1	C	226	THR
1	C	234	ILE
1	C	260	VAL
1	C	284	VAL
1	C	292	LEU
1	C	294	LYS
1	C	306	LEU
1	C	309	ILE
1	C	333	ILE
1	C	335	GLN
1	C	339	LEU
1	C	346	LEU
1	C	347	ILE
1	C	348	LEU
1	C	367	VAL
1	C	388	ILE
1	C	425	ASP
1	D	13	ARG
1	D	15	LEU
1	D	20	THR
1	D	27	GLN
1	D	36	THR
1	D	47	VAL
1	D	56	THR
1	D	62	VAL
1	D	163	SER
1	D	165	VAL
1	D	228	ILE
1	D	234	ILE
1	D	237	ILE
1	D	260	VAL
1	D	268	GLU
1	D	294	LYS
1	D	306	LEU
1	D	309	ILE
1	D	335	GLN
1	D	337	TYR

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Mol	Chain	Res	Type
1	D	342	THR
1	D	343	CYS
1	D	367	VAL
1	D	372	ILE
1	D	388	ILE
1	D	418	THR
1	D	431	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	71	HIS
1	A	95	GLN
1	A	156	ASN
1	A	241	HIS
1	A	331	HIS
1	A	417	HIS
1	B	52	GLN
1	B	71	HIS
1	B	73	ASN
1	B	95	GLN
1	B	139	HIS
1	B	156	ASN
1	B	171	HIS
1	B	179	ASN
1	B	241	HIS
1	B	368	GLN
1	B	393	GLN
1	B	458	GLN
1	B	531	ASN
1	C	27	GLN
1	C	71	HIS
1	C	95	GLN
1	C	156	ASN
1	C	241	HIS
1	C	275	GLN
1	C	331	HIS
1	C	335	GLN
1	C	368	GLN
1	C	375	ASN
1	D	27	GLN

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Mol	Chain	Res	Type
1	D	71	HIS
1	D	95	GLN
1	D	156	ASN
1	D	171	HIS
1	D	241	HIS
1	D	275	GLN
1	D	335	GLN
1	D	400	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	419/546 (76%)	-0.28	4 (0%) 79 54	30, 84, 159, 208	0
1	B	528/546 (96%)	-0.22	17 (3%) 50 29	46, 85, 145, 200	0
1	C	417/546 (76%)	-0.31	5 (1%) 76 50	49, 92, 160, 207	0
1	D	416/546 (76%)	-0.31	6 (1%) 73 46	51, 87, 160, 191	0
All	All	1780/2184 (81%)	-0.28	32 (1%) 67 40	30, 87, 157, 208	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	GLY	5.7
1	D	347	ILE	4.4
1	B	510	LEU	4.3
1	A	337	TYR	4.1
1	B	509	HIS	3.6
1	A	347	ILE	3.5
1	D	363	PRO	3.3
1	C	363	PRO	3.3
1	C	337	TYR	3.3
1	B	337	TYR	3.2
1	D	337	TYR	3.1
1	B	513	GLY	3.0
1	D	432	VAL	3.0
1	B	347	ILE	3.0
1	C	347	ILE	3.0
1	B	472	ASP	2.9
1	C	333	ILE	2.7
1	B	427	ASP	2.5
1	C	432	VAL	2.5
1	B	449	PRO	2.5
1	A	336	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	342	THR	2.5
1	B	539	ARG	2.3
1	B	468	ILE	2.3
1	D	424	TYR	2.3
1	A	433	VAL	2.2
1	B	478	LEU	2.2
1	B	338	GLY	2.1
1	B	345	ALA	2.1
1	B	512	GLY	2.1
1	D	388	ILE	2.1
1	B	480	SER	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.