



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:24 AM UTC

PDB ID : 7XHP / pdb_00007xhp
Title : Structure of a Glucose 6-Phosphate Dehydrogenase from Zymomonas mobilis
Authors : Meng, D.D.; Liu, M.X.; Liu, W.D.; You, C.
Deposited on : 2022-04-09
Resolution : 2.78 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

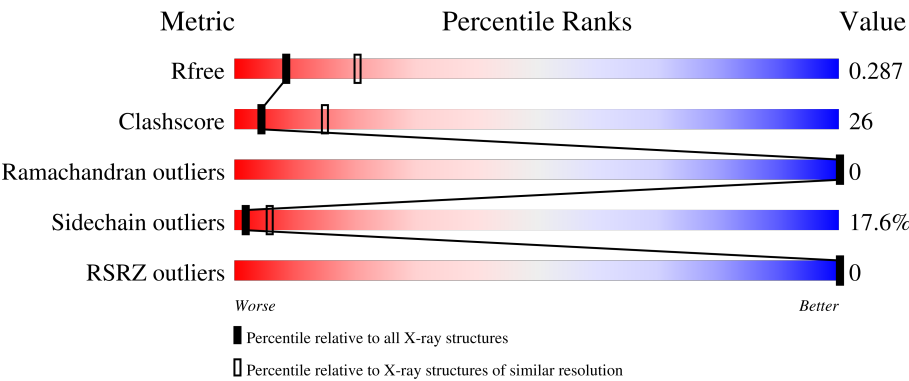
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	493	
1	B	493	
1	C	493	
1	D	493	
1	E	493	

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Mol	Chain	Length	Quality of chain
1	F	493	48% 41% 8%
1	G	493	45% 41% 9% 6%
1	H	493	51% 40% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26350 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 Glucose 6-Phosphate Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3319	2106	565	638	10			
1	B	461	Total	C	N	O	S	0	0	0
			3513	2235	601	666	11			
1	C	345	Total	C	N	O	S	0	0	0
			2684	1716	468	493	7			
1	D	361	Total	C	N	O	S	0	0	0
			2750	1749	486	508	7			
1	E	446	Total	C	N	O	S	0	0	0
			3324	2116	567	631	10			
1	F	480	Total	C	N	O	S	0	0	0
			3628	2305	620	692	11			
1	G	465	Total	C	N	O	S	0	0	0
			3521	2243	598	669	11			
1	H	474	Total	C	N	O	S	0	0	0
			3499	2224	591	674	10			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		
2	B	12	Total	O	0	0
			12	12		
2	C	11	Total	O	0	0
			11	11		
2	D	10	Total	O	0	0
			10	10		
2	E	8	Total	O	0	0
			8	8		
2	F	22	Total	O	0	0
			22	22		

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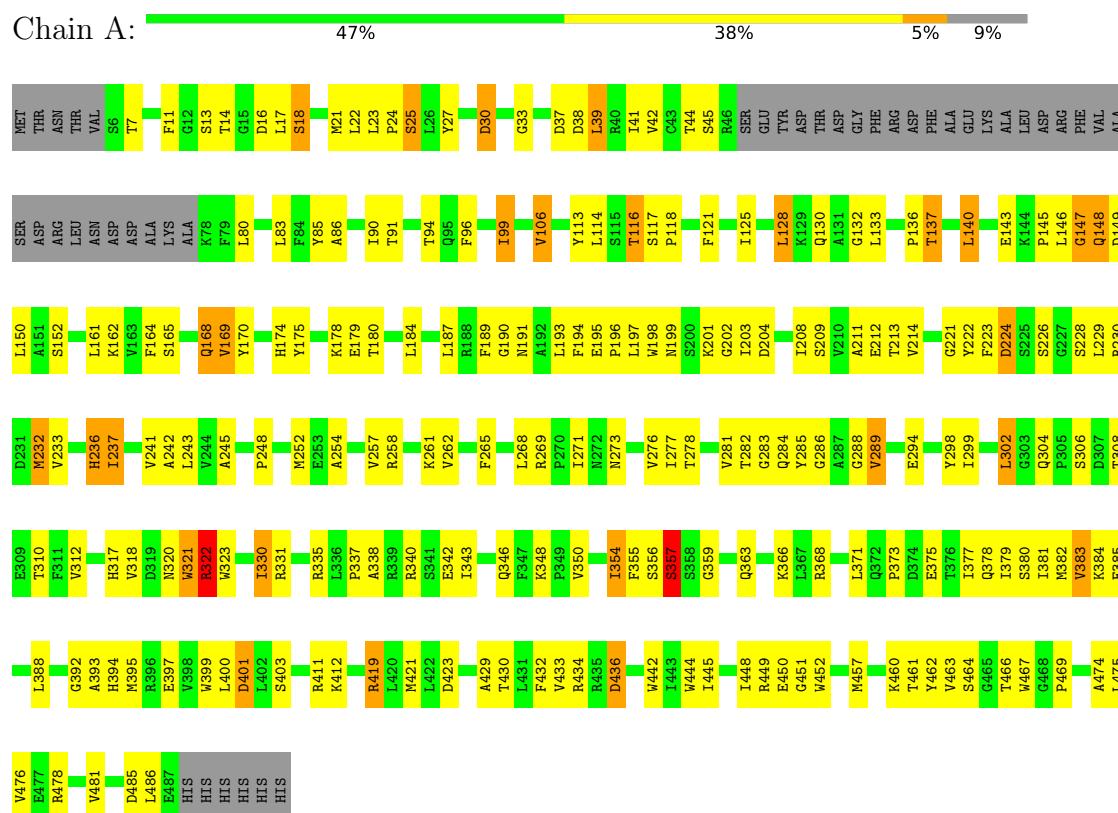
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	19	Total	O	0	0
			19	19		
2	H	13	Total	O	0	0
			13	13		

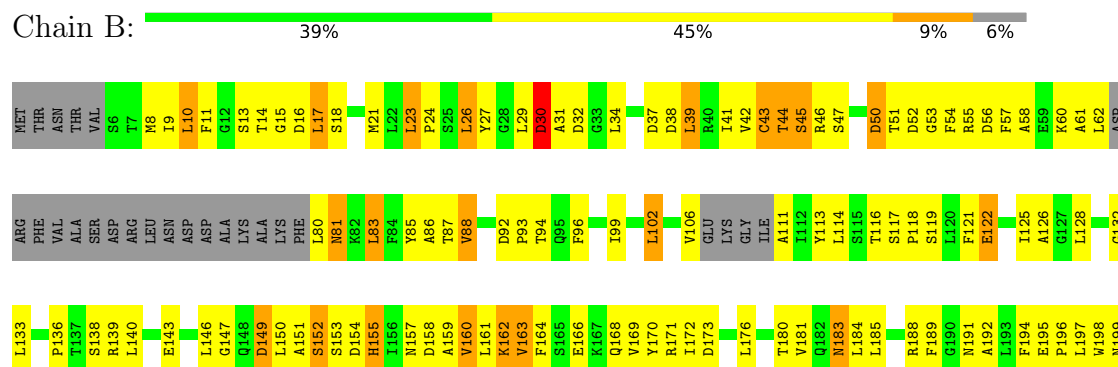
3 Residue-property plots

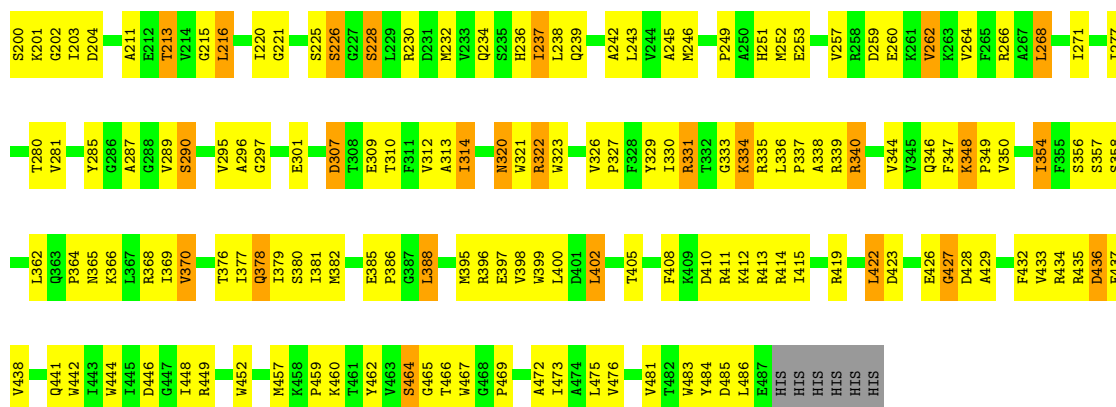
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glucose 6-Phosphate Dehydrogenase

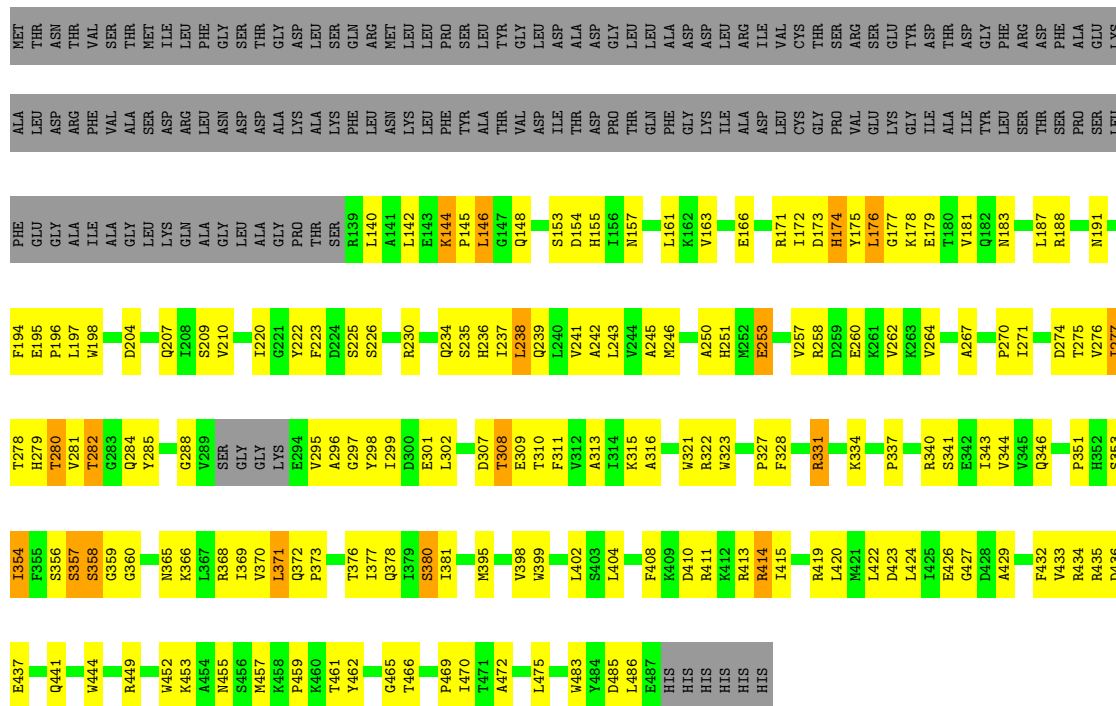


• Molecule 1: Glucose 6-Phosphate Dehydrogenase

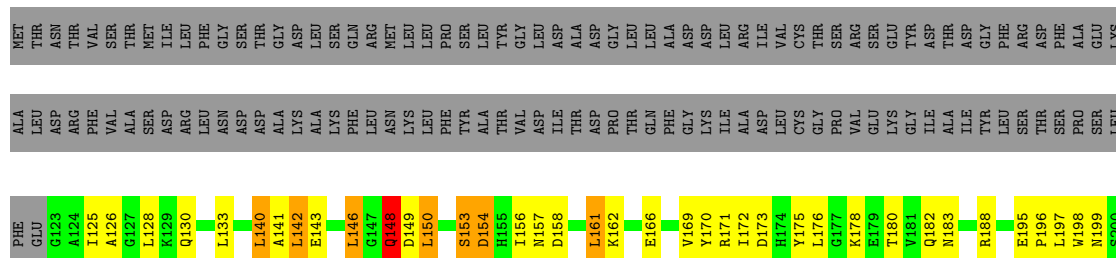


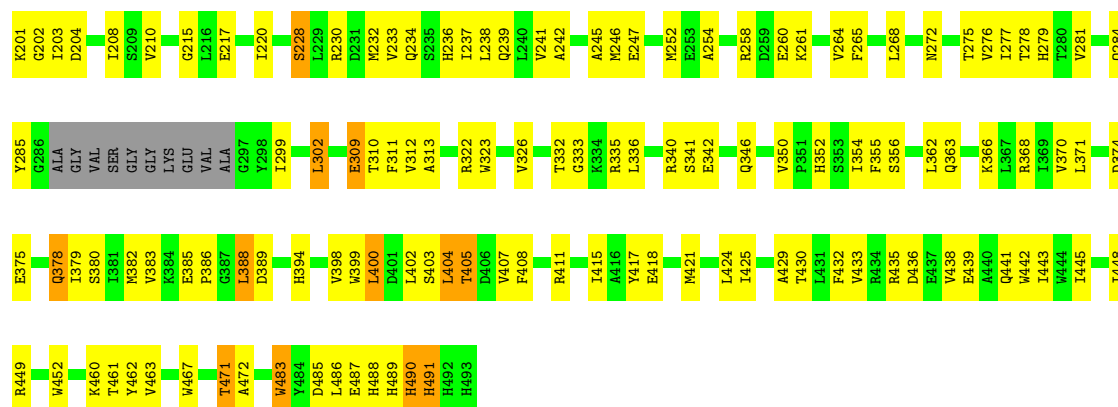


• Molecule 1: Glucose 6-Phosphate Dehydrogenase



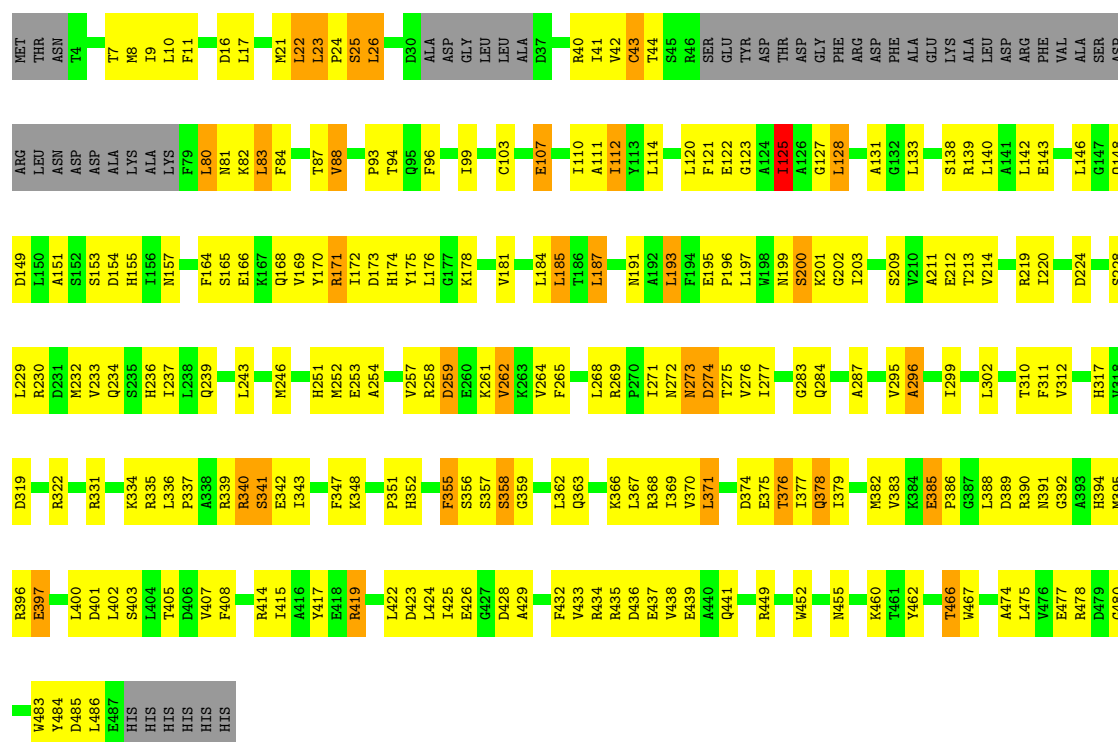
• Molecule 1: Glucose 6-Phosphate Dehydrogenase





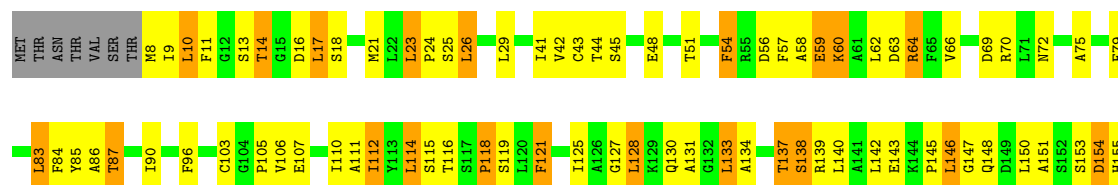
• Molecule 1: Glucose 6-Phosphate Dehydrogenase

Chain E: 45% 39% 6% 10%

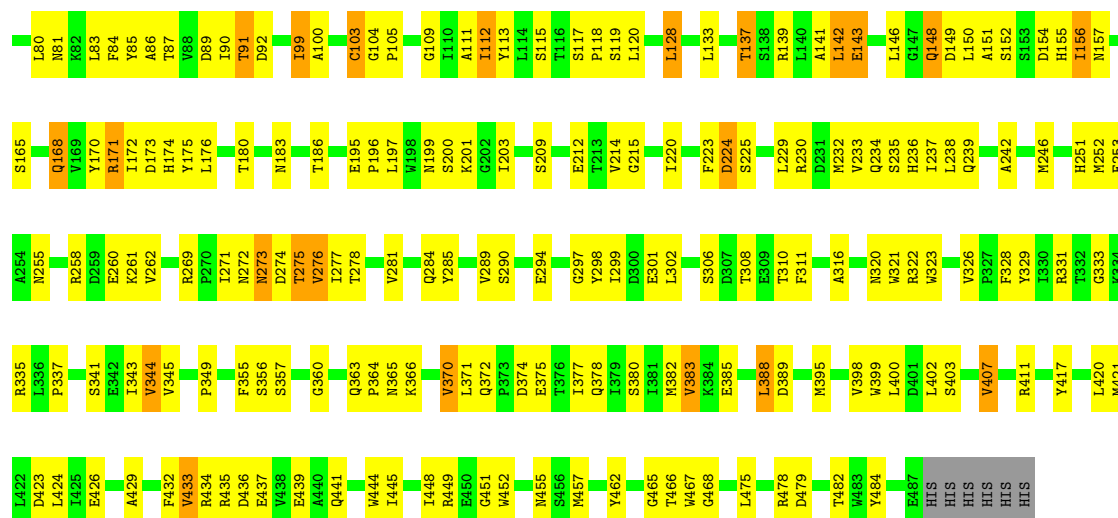


• Molecule 1: Glucose 6-Phosphate Dehydrogenase

Chain F: 48% 41% 8% 3%







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.61Å 101.07Å 321.07Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	78.18 – 2.78 78.18 – 2.78	Depositor EDS
% Data completeness (in resolution range)	90.8 (78.18-2.78) 89.5 (78.18-2.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.73 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.233 , 0.289 0.248 , 0.287	Depositor DCC
R_{free} test set	5876 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 96.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.439 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	0 of 118119 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26350	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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	0.62	0/3390	1.03	11/4634 (0.2%)
1	B	0.74	0/3586	1.18	8/4881 (0.2%)
1	C	0.46	0/2744	0.79	3/3733 (0.1%)
1	D	0.53	0/2817	0.92	2/3844 (0.1%)
1	E	0.68	0/3396	1.09	9/4637 (0.2%)
1	F	0.61	0/3706	1.01	8/5049 (0.2%)
1	G	0.64	0/3594	1.08	16/4894 (0.3%)
1	H	0.49	0/3575	0.83	0/4886
All	All	0.61	0/26808	1.01	57/36558 (0.2%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	ASP	N-CA-C	-10.68	100.53	114.31
1	G	416	ALA	N-CA-C	9.03	121.12	111.28
1	E	148	GLN	N-CA-C	-8.58	104.84	114.62
1	G	101	ASP	N-CA-C	-8.06	102.49	111.28
1	D	148	GLN	N-CA-C	-7.93	102.89	114.39
1	E	88	VAL	N-CA-C	7.61	119.30	111.00
1	B	136	PRO	N-CA-C	-7.10	103.67	113.53
1	F	148	GLN	N-CA-C	-6.93	104.43	113.17
1	G	219	ARG	N-CA-C	-6.89	103.27	113.61
1	F	145	PRO	N-CA-C	-6.84	100.50	111.03
1	B	427	GLY	N-CA-C	6.72	119.63	110.69
1	G	469	PRO	N-CA-C	-6.65	101.44	111.41
1	G	469	PRO	N-CA-CB	6.64	110.36	103.38
1	A	357	SER	N-CA-C	-6.58	105.13	113.02
1	G	102	LEU	N-CA-C	-6.49	99.14	109.59
1	E	125	ILE	N-CA-C	-6.46	106.44	112.83
1	G	121	PHE	CB-CA-C	-6.25	100.42	110.79
1	B	31	ALA	N-CA-C	6.20	118.04	111.28
1	D	228	SER	N-CA-C	-6.16	105.80	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	427	GLY	N-CA-C	6.04	119.26	110.63
1	G	359	GLY	N-CA-C	-6.00	106.81	115.27
1	A	147	GLY	CA-C-O	-5.98	118.10	122.23
1	A	221	GLY	N-CA-C	-5.91	108.05	115.08
1	A	16	ASP	CB-CA-C	-5.88	109.81	116.63
1	F	156	ILE	N-CA-C	-5.84	104.66	110.62
1	E	93	PRO	N-CA-C	-5.82	105.44	113.53
1	C	359	GLY	N-CA-C	-5.75	107.31	115.30
1	A	222	TYR	N-CA-C	-5.71	106.45	113.41
1	F	138	SER	N-CA-C	5.67	118.46	110.23
1	A	322	ARG	N-CA-C	-5.63	106.76	113.97
1	B	15	GLY	N-CA-C	5.62	117.94	111.36
1	G	270	PRO	N-CA-C	5.62	120.02	111.19
1	F	66	VAL	N-CA-C	-5.55	101.64	109.63
1	E	296	ALA	CA-C-N	-5.54	117.36	122.29
1	E	296	ALA	C-N-CA	-5.54	117.36	122.29
1	G	49	TYR	CB-CA-C	-5.50	102.24	110.88
1	B	221	GLY	N-CA-C	-5.50	108.06	115.21
1	C	145	PRO	CB-CA-C	-5.49	105.70	112.89
1	G	414	ARG	N-CA-C	5.45	117.72	110.53
1	A	130	GLN	N-CA-C	-5.43	105.36	111.28
1	G	6	SER	CA-C-N	-5.41	115.48	123.05
1	G	6	SER	C-N-CA	-5.41	115.48	123.05
1	G	37	ASP	N-CA-C	-5.41	106.61	114.12
1	A	147	GLY	N-CA-C	5.40	118.34	112.29
1	B	132	GLY	N-CA-C	-5.38	107.69	115.27
1	B	147	GLY	N-CA-C	5.36	118.54	110.18
1	E	123	GLY	CA-C-N	-5.32	115.89	123.03
1	E	123	GLY	C-N-CA	-5.32	115.89	123.03
1	F	486	LEU	CB-CA-C	-5.28	110.50	116.63
1	F	105	PRO	N-CA-C	-5.25	101.64	112.47
1	F	118	PRO	CB-CA-C	-5.22	105.06	111.64
1	G	192	ALA	N-CA-C	5.15	116.90	111.28
1	A	37	ASP	CA-C-N	-5.15	115.84	123.05
1	A	37	ASP	C-N-CA	-5.15	115.84	123.05
1	A	137	THR	N-CA-C	-5.13	102.46	110.10
1	G	412	LYS	N-CA-C	5.08	117.66	110.50
1	E	219	ARG	N-CA-C	5.07	116.81	111.28

There are no chirality outliers.

There are no planarity outliers.

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	3319	0	3109	158	0
1	B	3513	0	3417	216	0
1	C	2684	0	2635	130	0
1	D	2750	0	2611	157	0
1	E	3324	0	3150	181	0
1	F	3628	0	3471	193	0
1	G	3521	0	3377	217	0
1	H	3499	0	3273	185	0
2	A	17	0	0	2	0
2	B	12	0	0	0	0
2	C	11	0	0	4	0
2	D	10	0	0	0	0
2	E	8	0	0	1	0
2	F	22	0	0	5	0
2	G	19	0	0	1	0
2	H	13	0	0	1	0
All	All	26350	0	25043	1356	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 26.

All (1356) 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:F:8:MET:HG2	1:F:111:ALA:HB3	1.43	1.00
1:H:100:ALA:HB2	1:H:133:LEU:HD11	1.45	0.96
1:B:215:GLY:HA3	1:B:335:ARG:HH11	1.32	0.95
1:G:125:ILE:HG21	1:G:160:VAL:HA	1.49	0.94
1:G:6:SER:HA	1:G:39:LEU:HD13	1.49	0.93
1:A:13:SER:HA	1:A:18:SER:HB2	1.50	0.93
1:A:363:GLN:H	1:A:382:MET:HE2	1.34	0.92
1:H:285:TYR:HB3	1:H:298:TYR:HB2	1.51	0.92
1:G:125:ILE:HG12	1:G:160:VAL:HG13	1.52	0.92
1:G:340:ARG:HG3	1:G:373:PRO:HD2	1.51	0.90
1:C:411:ARG:HD2	1:D:385:GLU:HG2	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:GLY:HA3	1:F:153:SER:HB2	1.54	0.89
1:G:216:LEU:HD23	1:G:334:LYS:HD2	1.54	0.89
1:A:271:ILE:HB	1:A:448:ILE:HG12	1.57	0.87
1:H:143:GLU:HG2	1:H:172:ILE:HB	1.56	0.87
1:F:319:ASP:HB3	1:G:352:HIS:HE1	1.41	0.86
1:H:272:ASN:HB3	1:H:275:THR:HG23	1.60	0.84
1:A:224:ASP:HA	1:A:308:THR:HG21	1.61	0.82
1:A:233:VAL:HA	1:A:237:ILE:HG13	1.60	0.82
1:E:22:LEU:HA	1:E:25:SER:HB3	1.61	0.82
1:E:166:GLU:HA	1:E:169:VAL:HG12	1.60	0.82
1:F:419:ARG:HE	1:F:431:LEU:HD11	1.45	0.81
1:C:354:ILE:HB	1:D:252:MET:HG2	1.60	0.81
1:G:6:SER:HA	1:G:39:LEU:CD1	2.10	0.81
1:E:211:ALA:HB1	1:E:336:LEU:HB2	1.63	0.81
1:E:283:GLY:H	1:E:311:PHE:HB3	1.43	0.79
1:D:220:ILE:HG12	1:D:302:LEU:HD21	1.62	0.79
1:A:452:TRP:HB2	1:A:457:MET:HB2	1.65	0.79
1:A:476:VAL:HB	1:A:481:VAL:HB	1.65	0.79
1:F:216:LEU:HD12	1:F:220:ILE:HD13	1.65	0.78
1:C:411:ARG:HG3	1:D:386:PRO:HD2	1.66	0.77
1:G:5:VAL:HG11	1:G:111:ALA:HB2	1.66	0.77
1:C:296:ALA:HB3	1:C:301:GLU:HG3	1.66	0.77
1:B:246:MET:HE3	1:B:260:GLU:HB2	1.64	0.77
1:G:14:THR:CG2	1:G:45:SER:OG	2.33	0.77
1:C:452:TRP:HB2	1:C:457:MET:HB2	1.66	0.77
1:A:39:LEU:HD11	1:A:41:ILE:HG12	1.66	0.76
1:G:207:GLN:HE22	1:G:484:TYR:H	1.31	0.76
1:G:216:LEU:HD12	1:G:220:ILE:HG23	1.70	0.74
1:H:224:ASP:O	1:H:308:THR:HG21	1.88	0.74
1:F:166:GLU:OE1	1:F:171:ARG:NH2	2.21	0.74
1:G:331:ARG:NH2	2:G:501:HOH:O	2.20	0.74
1:H:77:ALA:HA	1:H:80:LEU:HB2	1.68	0.74
1:G:14:THR:HG22	1:G:45:SER:OG	1.88	0.74
1:A:320:ASN:O	1:A:321:TRP:HB3	1.88	0.73
1:G:429:ALA:HB1	1:G:432:PHE:HD2	1.52	0.73
1:E:272:ASN:O	1:E:275:THR:N	2.20	0.73
1:G:176:LEU:HB3	1:G:431:LEU:HD22	1.69	0.73
1:A:284:GLN:NE2	1:A:308:THR:O	2.22	0.73
1:G:299:ILE:HD11	1:G:306:SER:HB3	1.71	0.73
1:B:45:SER:O	1:B:87:THR:HG23	1.88	0.73
1:F:271:ILE:HG23	1:F:275:THR:HB	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ASP:HA	1:C:435:ARG:HH22	1.54	0.72
1:H:235:SER:O	1:H:239:GLN:HG2	1.88	0.72
1:E:388:LEU:HD22	1:F:419:ARG:HB2	1.69	0.72
1:E:422:LEU:HA	1:E:425:ILE:HD12	1.72	0.72
1:A:411:ARG:NH2	1:B:386:PRO:O	2.22	0.72
1:F:229:LEU:HD21	1:F:445:ILE:HD12	1.72	0.72
1:G:419:ARG:HG3	1:H:388:LEU:HD22	1.72	0.72
1:F:475:LEU:HD12	1:F:478:ARG:HH12	1.55	0.71
1:E:254:ALA:HB2	1:E:428:ASP:HB3	1.72	0.71
1:G:389:ASP:HB2	1:G:392:GLY:O	1.91	0.71
1:E:138:SER:OG	1:E:168:GLN:HB3	1.90	0.71
1:F:56:ASP:O	1:F:59:GLU:HB3	1.91	0.70
1:D:210:VAL:HG22	1:D:341:SER:HB3	1.73	0.70
1:B:8:MET:HB3	1:B:39:LEU:HD11	1.73	0.70
1:G:258:ARG:HD2	1:G:430:THR:HA	1.73	0.70
1:H:289:VAL:HA	1:H:294:GLU:HA	1.72	0.70
1:B:385:GLU:HG3	1:B:386:PRO:HD2	1.72	0.70
1:F:48:GLU:HA	1:F:87:THR:CB	2.20	0.70
1:H:173:ASP:OD2	1:H:239:GLN:NE2	2.24	0.70
1:E:271:ILE:HG22	1:E:276:VAL:HG22	1.72	0.70
1:B:140:LEU:N	1:B:168:GLN:O	2.24	0.70
1:F:299:ILE:HD11	1:F:306:SER:OG	1.90	0.70
1:A:254:ALA:HA	1:A:430:THR:HG22	1.73	0.70
1:B:111:ALA:HA	1:B:139:ARG:O	1.92	0.70
1:B:287:ALA:HB2	1:B:297:GLY:N	2.07	0.70
1:H:89:ASP:HB3	1:H:92:ASP:HB2	1.74	0.69
1:B:369:ILE:HG12	1:B:377:ILE:HG23	1.73	0.69
1:E:359:GLY:HA3	1:E:394:HIS:HD2	1.57	0.69
1:A:321:TRP:HB2	1:D:352:HIS:HB3	1.75	0.69
1:A:354:ILE:HD12	1:B:252:MET:HG2	1.74	0.69
1:G:284:GLN:N	1:G:460:LYS:O	2.24	0.69
1:A:113:TYR:OH	1:A:145:PRO:HD2	1.93	0.69
1:A:13:SER:HA	1:A:18:SER:CB	2.23	0.68
1:C:429:ALA:HB1	1:C:432:PHE:CD1	2.29	0.68
1:H:284:GLN:HE21	1:H:298:TYR:HD2	1.42	0.68
1:A:30:ASP:HA	1:A:33:GLY:O	1.94	0.68
1:H:273:ASN:O	1:H:455:ASN:ND2	2.26	0.68
1:B:337:PRO:HG2	1:B:467:TRP:CD1	2.27	0.68
1:C:315:LYS:HE2	1:C:327:PRO:HB3	1.74	0.68
1:A:384:LYS:HA	1:A:395:MET:HG2	1.76	0.68
1:G:207:GLN:HE22	1:G:484:TYR:N	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:365:ASN:ND2	1:H:380:SER:O	2.27	0.68
1:G:146:LEU:O	1:G:156:ILE:HD12	1.93	0.67
1:H:417:TYR:HA	1:H:420:LEU:HD12	1.77	0.67
1:B:154:ASP:CG	1:B:435:ARG:HH22	2.01	0.67
1:A:190:GLY:HA2	1:B:362:LEU:HD23	1.76	0.67
1:B:473:ILE:HG12	1:G:289:VAL:HG21	1.77	0.67
1:D:125:ILE:HD12	1:D:125:ILE:H	1.60	0.67
1:E:385:GLU:H	1:E:395:MET:HA	1.59	0.67
1:F:415:ILE:HG22	1:F:418:GLU:HG2	1.76	0.67
1:A:7:THR:HG23	1:A:42:VAL:H	1.59	0.67
1:B:43:CYS:HB2	1:B:85:TYR:HD1	1.58	0.67
1:B:226:SER:O	1:B:230:ARG:HB2	1.95	0.66
1:D:368:ARG:HH21	1:D:370:VAL:HG21	1.61	0.66
1:E:10:LEU:N	1:E:42:VAL:O	2.28	0.66
1:F:48:GLU:HA	1:F:87:THR:HB	1.77	0.66
1:F:337:PRO:HG2	1:F:467:TRP:CD1	2.30	0.66
1:G:276:VAL:HG21	1:G:452:TRP:HB3	1.76	0.66
1:B:55:ARG:HA	1:B:83:LEU:HD22	1.76	0.66
1:C:341:SER:N	1:C:372:GLN:O	2.28	0.66
1:H:258:ARG:NH1	1:H:432:PHE:O	2.29	0.66
1:H:251:HIS:ND1	1:H:253:GLU:OE2	2.29	0.66
1:A:44:THR:HA	1:A:86:ALA:O	1.96	0.66
1:E:139:ARG:HA	1:E:168:GLN:HA	1.77	0.66
1:E:170:TYR:CE2	1:E:424:LEU:HA	2.31	0.66
1:E:41:ILE:HG13	1:E:82:LYS:CB	2.26	0.66
1:G:112:ILE:HB	1:G:140:LEU:HG	1.76	0.66
1:G:140:LEU:O	1:G:170:TYR:N	2.21	0.65
1:G:337:PRO:HG2	1:G:467:TRP:CD1	2.30	0.65
1:F:259:ASP:OD1	1:F:434:ARG:NH2	2.23	0.65
1:A:359:GLY:HA3	1:A:393:ALA:O	1.97	0.65
1:G:284:GLN:NE2	1:G:308:THR:O	2.28	0.65
1:B:369:ILE:HG23	1:B:377:ILE:HG12	1.79	0.65
1:A:342:GLU:OE1	1:A:368:ARG:NH1	2.30	0.65
1:G:408:PHE:HB3	1:G:411:ARG:HG3	1.79	0.65
1:H:104:GLY:N	1:H:105:PRO:HD3	2.12	0.65
1:A:357:SER:HB2	1:A:392:GLY:HA2	1.78	0.65
1:H:21:MET:O	1:H:22:LEU:HD23	1.96	0.65
1:B:215:GLY:HA3	1:B:335:ARG:NH1	2.09	0.65
1:D:239:GLN:HG3	1:D:265:PHE:HZ	1.62	0.65
1:F:54:PHE:O	1:F:58:ALA:HB3	1.96	0.65
1:H:466:THR:HG23	1:H:468:GLY:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ARG:HB3	1:D:386:PRO:HB2	1.78	0.64
1:A:21:MET:O	1:A:24:PRO:HD2	1.97	0.64
1:E:175:TYR:HA	1:E:178:LYS:HE2	1.79	0.64
1:G:171:ARG:O	1:G:433:VAL:N	2.20	0.64
1:B:188:ARG:NH1	1:B:243:LEU:O	2.31	0.64
1:B:295:VAL:HB	1:B:335:ARG:NH2	2.12	0.64
1:H:251:HIS:CD2	1:H:252:MET:H	2.16	0.64
1:F:14:THR:HG22	1:F:45:SER:HB2	1.79	0.64
1:G:26:LEU:HA	1:G:29:LEU:HD12	1.80	0.64
1:H:355:PHE:C	1:H:357:SER:H	2.04	0.64
1:A:262:VAL:HG11	1:A:436:ASP:HB2	1.78	0.64
1:H:7:THR:HG23	1:H:103:CYS:SG	2.38	0.64
1:B:365:ASN:ND2	1:B:380:SER:O	2.31	0.64
1:C:277:ILE:HG12	1:C:455:ASN:HD22	1.61	0.64
1:F:155:HIS:HA	1:F:158:ASP:HB2	1.79	0.64
1:G:6:SER:H	1:G:109:GLY:HA3	1.63	0.64
1:G:386:PRO:O	1:H:411:ARG:NH2	2.30	0.64
1:A:140:LEU:HD13	1:A:169:VAL:HG23	1.79	0.64
1:E:251:HIS:HD1	1:E:252:MET:H	1.46	0.64
1:G:148:GLN:O	1:G:230:ARG:NH1	2.30	0.63
1:E:211:ALA:O	1:E:339:ARG:HA	1.98	0.63
1:C:337:PRO:HG3	1:C:465:GLY:HA2	1.80	0.63
1:A:299:ILE:HG22	1:A:306:SER:H	1.64	0.63
1:F:201:LYS:HE2	1:G:201:LYS:O	1.99	0.63
1:G:154:ASP:HA	1:G:435:ARG:HH12	1.64	0.63
1:G:429:ALA:HB1	1:G:432:PHE:CD2	2.33	0.63
1:A:388:LEU:HD23	1:B:419:ARG:HA	1.81	0.63
1:B:436:ASP:OD1	1:B:436:ASP:N	2.25	0.63
1:F:96:PHE:HD2	1:F:127:GLY:HA3	1.63	0.63
1:G:258:ARG:NH2	1:G:432:PHE:O	2.32	0.63
1:A:191:ASN:HB2	1:A:194:PHE:CE2	2.33	0.63
1:F:212:GLU:HA	1:F:339:ARG:HA	1.80	0.63
1:H:99:ILE:HG13	1:H:100:ALA:N	2.13	0.63
1:G:54:PHE:HA	1:G:57:PHE:HB3	1.81	0.63
1:H:235:SER:HG	1:H:236:HIS:HD1	1.47	0.63
1:A:128:LEU:O	1:A:132:GLY:N	2.31	0.62
1:C:277:ILE:HG12	1:C:455:ASN:ND2	2.13	0.62
1:A:285:TYR:HB3	1:A:298:TYR:HB2	1.81	0.62
1:H:378:GLN:HB2	1:H:399:TRP:CE3	2.35	0.62
1:C:250:ALA:O	1:D:352:HIS:NE2	2.31	0.62
1:E:21:MET:O	1:E:22:LEU:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:VAL:HG12	1:E:261:LYS:HD2	1.80	0.62
1:F:299:ILE:CD1	1:F:306:SER:OG	2.47	0.62
1:B:203:ILE:HG23	1:B:346:GLN:O	1.99	0.62
1:D:311:PHE:HE1	1:D:336:LEU:HD11	1.64	0.62
1:A:191:ASN:HB2	1:A:194:PHE:HE2	1.65	0.62
1:D:277:ILE:HG23	1:D:278:THR:HG23	1.82	0.62
1:F:110:ILE:CB	1:F:138:SER:HA	2.30	0.62
1:F:153:SER:HA	1:F:156:ILE:HD12	1.82	0.62
1:G:21:MET:C	1:G:24:PRO:HD2	2.25	0.62
1:F:195:GLU:N	1:F:196:PRO:HD2	2.14	0.62
1:H:80:LEU:HD23	1:H:83:LEU:HD12	1.80	0.62
1:H:142:LEU:HB2	1:H:146:LEU:HD11	1.82	0.62
1:A:106:VAL:O	1:A:136:PRO:HG3	2.00	0.62
1:A:213:THR:HG23	1:A:214:VAL:HG13	1.82	0.62
1:F:256:ALA:O	1:F:260:GLU:HG2	2.00	0.62
1:E:474:ALA:O	1:E:478:ARG:N	2.28	0.61
1:F:233:VAL:HA	1:F:237:ILE:HB	1.80	0.61
1:H:109:GLY:HA2	1:H:137:THR:OG1	2.00	0.61
1:A:236:HIS:H	1:A:236:HIS:CD2	2.17	0.61
1:F:54:PHE:CD2	1:F:85:TYR:HB2	2.36	0.61
1:A:245:ALA:O	1:A:323:TRP:NE1	2.33	0.61
1:D:230:ARG:HD2	1:D:442:TRP:HZ3	1.65	0.61
1:E:341:SER:O	1:E:370:VAL:HA	2.01	0.61
1:H:320:ASN:OD1	1:H:323:TRP:N	2.27	0.61
1:E:41:ILE:HD12	1:E:83:LEU:HD23	1.83	0.61
1:H:273:ASN:O	1:H:276:VAL:HG12	2.00	0.61
1:A:18:SER:HA	1:A:22:LEU:HB2	1.82	0.61
1:B:10:LEU:HB3	1:B:42:VAL:O	2.00	0.61
1:F:134:ALA:HB1	1:F:163:VAL:HG21	1.83	0.61
1:G:146:LEU:HD12	1:G:438:VAL:HG13	1.82	0.61
1:B:170:TYR:HB3	1:B:432:PHE:CD2	2.36	0.60
1:F:215:GLY:HA2	1:F:334:LYS:HD2	1.83	0.60
1:B:50:ASP:HB2	1:B:53:GLY:H	1.64	0.60
1:B:249:PRO:HG3	1:B:257:VAL:HG22	1.82	0.60
1:H:128:LEU:HG	1:H:133:LEU:HB2	1.83	0.60
1:H:175:TYR:CD2	1:H:236:HIS:HB3	2.36	0.60
1:A:191:ASN:OD1	1:B:382:MET:N	2.32	0.60
1:E:203:ILE:HA	1:E:347:PHE:HA	1.83	0.60
1:F:452:TRP:HB2	1:F:457:MET:HE3	1.82	0.60
1:H:18:SER:O	1:H:23:LEU:HB2	2.01	0.60
1:B:26:LEU:HG	1:B:61:ALA:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:VAL:HG21	1:B:436:ASP:HB2	1.82	0.60
1:G:122:GLU:HG2	1:G:159:ALA:HB3	1.82	0.60
1:A:114:LEU:HD23	1:A:121:PHE:HA	1.83	0.60
1:A:258:ARG:NH1	1:A:432:PHE:O	2.34	0.60
1:B:271:ILE:HB	1:B:448:ILE:HG12	1.83	0.60
1:B:460:LYS:HD3	1:B:469:PRO:HB2	1.83	0.60
1:F:85:TYR:CG	1:F:86:ALA:N	2.70	0.60
1:E:484:TYR:CE1	1:E:486:LEU:HB3	2.37	0.60
1:G:164:PHE:HB3	1:G:168:GLN:HB2	1.83	0.60
1:D:171:ARG:HE	1:D:438:VAL:HG11	1.67	0.60
1:A:288:GLY:HA3	1:A:463:VAL:HG13	1.83	0.60
1:C:166:GLU:OE2	1:C:171:ARG:NH2	2.34	0.60
1:D:436:ASP:OD1	1:D:436:ASP:N	2.34	0.60
1:E:243:LEU:HA	1:E:246:MET:HE2	1.84	0.60
1:H:378:GLN:HB2	1:H:399:TRP:HE3	1.65	0.60
1:E:178:LYS:HB2	1:E:181:VAL:HG23	1.84	0.60
1:B:143:GLU:HB3	1:B:172:ILE:HD12	1.83	0.59
1:C:154:ASP:OD1	1:C:435:ARG:NH2	2.34	0.59
1:E:127:GLY:O	1:E:131:ALA:N	2.35	0.59
1:E:170:TYR:HB3	1:E:432:PHE:CD2	2.36	0.59
1:F:336:LEU:HD13	1:F:467:TRP:CZ3	2.36	0.59
1:G:5:VAL:HA	1:G:109:GLY:HA3	1.84	0.59
1:D:195:GLU:HA	1:D:198:TRP:HB2	1.84	0.59
1:E:400:LEU:HD23	1:F:402:LEU:HB3	1.84	0.59
1:B:160:VAL:HG13	1:B:164:PHE:HD2	1.67	0.59
1:H:269:ARG:C	1:H:444:TRP:HE1	2.10	0.59
1:H:466:THR:O	1:H:467:TRP:HB2	2.02	0.59
1:E:9:ILE:HB	1:E:112:ILE:HG23	1.85	0.59
1:F:205:HIS:HB3	1:F:327:PRO:HG2	1.83	0.59
1:G:281:VAL:O	1:G:312:VAL:HA	2.01	0.59
1:D:154:ASP:HA	1:D:157:ASN:HB2	1.85	0.59
1:D:284:GLN:HB3	1:D:461:THR:HA	1.84	0.59
1:G:230:ARG:HA	1:G:234:GLN:HB2	1.84	0.59
1:D:435:ARG:HA	1:D:438:VAL:HG22	1.85	0.59
1:D:404:LEU:HD22	1:D:408:PHE:HE2	1.67	0.59
1:H:197:LEU:O	1:H:203:ILE:HG13	2.03	0.59
1:B:117:SER:HB2	1:B:118:PRO:HD2	1.85	0.59
1:F:319:ASP:HB3	1:G:352:HIS:CE1	2.30	0.59
1:H:29:LEU:O	1:H:34:LEU:HB2	2.03	0.59
1:H:76:LYS:O	1:H:80:LEU:N	2.33	0.59
1:H:273:ASN:HA	1:H:451:GLY:CA	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:408:PHE:HB3	1:G:411:ARG:CG	2.32	0.58
1:A:175:TYR:HA	1:A:178:LYS:HD2	1.84	0.58
1:C:271:ILE:HG22	1:C:276:VAL:HG22	1.85	0.58
1:F:187:LEU:O	1:F:191:ASN:ND2	2.34	0.58
1:A:208:ILE:HG12	1:A:343:ILE:HG23	1.84	0.58
1:A:350:VAL:HG12	1:B:192:ALA:HB2	1.84	0.58
1:B:151:ALA:O	1:B:155:HIS:HB3	2.03	0.58
1:C:285:TYR:CE1	1:C:298:TYR:HB2	2.38	0.58
1:C:315:LYS:NZ	2:C:502:HOH:O	2.35	0.58
1:E:466:THR:O	1:E:467:TRP:HB2	2.03	0.58
1:A:258:ARG:HA	1:A:261:LYS:HD3	1.85	0.58
1:G:156:ILE:O	1:G:160:VAL:HG23	2.04	0.58
1:A:463:VAL:HB	1:A:466:THR:HG21	1.86	0.58
1:H:274:ASP:O	1:H:277:ILE:HG22	2.03	0.58
1:G:153:SER:OG	1:G:442:TRP:NE1	2.37	0.58
1:E:10:LEU:O	1:E:44:THR:N	2.37	0.58
1:E:10:LEU:HD23	1:E:43:CYS:HB3	1.86	0.58
1:D:487:GLU:HA	1:D:490:HIS:CE1	2.39	0.58
1:G:280:THR:HG23	1:G:314:ILE:HG23	1.86	0.58
1:H:276:VAL:HG12	1:H:455:ASN:HD22	1.68	0.58
1:C:410:ASP:CG	1:C:411:ARG:HE	2.12	0.57
1:E:385:GLU:N	1:E:395:MET:HA	2.18	0.57
1:H:234:GLN:NE2	1:H:441:GLN:OE1	2.37	0.57
1:H:258:ARG:NH1	1:H:429:ALA:O	2.37	0.57
1:C:148:GLN:NE2	1:C:225:SER:O	2.37	0.57
1:D:483:TRP:HA	1:D:483:TRP:CE3	2.39	0.57
1:F:60:LYS:HB2	1:F:64:ARG:CZ	2.34	0.57
1:G:419:ARG:CG	1:H:388:LEU:HD22	2.34	0.57
1:B:242:ALA:HA	1:B:264:VAL:HG11	1.85	0.57
1:C:209:SER:HB2	1:C:331:ARG:NH2	2.20	0.57
1:H:156:ILE:HG13	1:H:157:ASN:N	2.18	0.57
1:A:165:SER:N	1:A:168:GLN:HG3	2.20	0.57
1:B:43:CYS:HB2	1:B:85:TYR:CD1	2.39	0.57
1:C:178:LYS:HB2	1:C:181:VAL:HG23	1.86	0.57
1:C:262:VAL:HG22	1:C:437:GLU:HG2	1.85	0.57
1:B:412:LYS:HG2	1:B:413:ARG:H	1.69	0.57
1:C:226:SER:HA	1:C:230:ARG:HE	1.69	0.57
1:G:146:LEU:HD11	1:G:234:GLN:HE22	1.68	0.57
1:F:434:ARG:O	1:F:438:VAL:HG23	2.05	0.57
1:H:322:ARG:HG2	1:H:323:TRP:CD1	2.40	0.57
1:E:23:LEU:HB2	1:E:24:PRO:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PRO:HD2	1:B:467:TRP:CD2	2.39	0.57
1:G:5:VAL:HG22	1:G:110:ILE:H	1.70	0.57
1:G:408:PHE:O	1:G:411:ARG:HB2	2.05	0.57
1:H:385:GLU:H	1:H:395:MET:HA	1.70	0.57
1:A:165:SER:H	1:A:168:GLN:HG3	1.70	0.57
1:B:336:LEU:HD13	1:B:467:TRP:HE3	1.68	0.57
1:D:449:ARG:HA	1:D:452:TRP:CD1	2.40	0.57
1:B:230:ARG:O	1:B:234:GLN:HG2	2.04	0.56
1:D:195:GLU:OE1	1:D:322:ARG:NH1	2.38	0.56
1:D:378:GLN:HB2	1:D:399:TRP:HE3	1.70	0.56
1:D:178:LYS:O	1:D:182:GLN:HG3	2.04	0.56
1:A:170:TYR:HE2	1:A:429:ALA:HB3	1.70	0.56
1:A:189:PHE:CD1	1:A:248:PRO:HB3	2.40	0.56
1:D:385:GLU:O	1:D:394:HIS:HB2	2.06	0.56
1:D:439:GLU:O	1:D:443:ILE:HG13	2.05	0.56
1:G:146:LEU:HD11	1:G:234:GLN:NE2	2.19	0.56
1:G:201:LYS:O	1:G:348:LYS:HD2	2.06	0.56
1:G:254:ALA:O	1:G:430:THR:HB	2.04	0.56
1:A:286:GLY:O	1:A:464:SER:OG	2.20	0.56
1:B:41:ILE:HD13	1:B:83:LEU:HD12	1.87	0.56
1:B:88:VAL:HG13	1:B:99:ILE:HD11	1.87	0.56
1:E:128:LEU:HG	1:E:164:PHE:HZ	1.71	0.56
1:F:146:LEU:HD12	1:F:234:GLN:HE22	1.71	0.56
1:F:340:ARG:HH12	1:F:485:ASP:CG	2.14	0.56
1:G:267:ALA:O	1:G:319:ASP:HB2	2.05	0.56
1:G:466:THR:O	1:G:467:TRP:HB2	2.03	0.56
1:B:158:ASP:O	1:B:162:LYS:HG2	2.05	0.56
1:B:170:TYR:HB3	1:B:432:PHE:CG	2.40	0.56
1:C:179:GLU:CD	1:D:386:PRO:HB3	2.31	0.56
1:E:402:LEU:HB2	1:F:400:LEU:HA	1.88	0.56
1:A:197:LEU:O	1:A:202:GLY:HA3	2.06	0.56
1:B:259:ASP:O	1:B:262:VAL:HG12	2.05	0.56
1:C:368:ARG:HG2	1:C:378:GLN:HG3	1.86	0.56
1:D:490:HIS:C	1:D:490:HIS:CD2	2.84	0.56
1:E:212:GLU:HA	1:E:339:ARG:HG3	1.86	0.56
1:E:276:VAL:HG11	1:E:452:TRP:HB3	1.86	0.56
1:F:23:LEU:N	1:F:24:PRO:HD2	2.21	0.56
1:F:423:ASP:HB3	1:F:429:ALA:HB2	1.87	0.56
1:G:140:LEU:N	1:G:168:GLN:O	2.38	0.56
1:B:321:TRP:CD1	1:C:351:PRO:HG2	2.41	0.56
1:C:246:MET:HE3	1:C:260:GLU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:TYR:O	1:D:418:GLU:HG2	2.04	0.56
1:G:384:LYS:N	1:H:186:THR:HG21	2.21	0.56
1:D:265:PHE:HA	1:D:268:LEU:HD12	1.87	0.56
1:E:233:VAL:HA	1:E:237:ILE:HB	1.88	0.56
1:F:223:PHE:HE2	1:F:310:THR:HG22	1.70	0.56
1:F:296:ALA:O	1:F:335:ARG:NH2	2.38	0.56
1:G:452:TRP:HB2	1:G:457:MET:HB2	1.88	0.56
1:A:90:ILE:HA	1:A:96:PHE:CZ	2.41	0.56
1:E:435:ARG:NH2	1:E:439:GLU:HG3	2.21	0.56
1:G:238:LEU:HD23	1:G:441:GLN:HG2	1.87	0.56
1:B:290:SER:HB2	1:B:295:VAL:HG11	1.86	0.55
1:E:234:GLN:NE2	1:E:441:GLN:OE1	2.39	0.55
1:E:317:HIS:HB3	1:E:319:ASP:OD1	2.06	0.55
1:H:302:LEU:HD23	1:H:306:SER:HB2	1.86	0.55
1:C:191:ASN:OD1	1:D:382:MET:N	2.32	0.55
1:C:226:SER:CA	1:C:230:ARG:HE	2.19	0.55
1:B:44:THR:HG22	1:B:88:VAL:HG22	1.88	0.55
1:C:210:VAL:HG22	1:C:341:SER:HB3	1.88	0.55
1:D:148:GLN:O	1:D:230:ARG:NH1	2.39	0.55
1:D:285:TYR:N	1:D:310:THR:OG1	2.40	0.55
1:G:51:THR:O	1:G:85:TYR:HB3	2.07	0.55
1:G:419:ARG:O	1:G:419:ARG:HG2	2.07	0.55
1:A:273:ASN:HB3	1:A:451:GLY:HA2	1.87	0.55
1:E:258:ARG:NH1	1:E:434:ARG:HB2	2.22	0.55
1:G:6:SER:N	1:G:109:GLY:HA3	2.22	0.55
1:B:378:GLN:HB2	1:B:399:TRP:CE3	2.41	0.55
1:D:340:ARG:NH1	1:D:368:ARG:HH22	2.04	0.55
1:G:336:LEU:HD13	1:G:467:TRP:CZ3	2.41	0.55
1:H:49:TYR:O	1:H:85:TYR:CE1	2.60	0.55
1:A:252:MET:HE2	1:A:252:MET:HA	1.87	0.55
1:D:128:LEU:HA	1:D:133:LEU:HD12	1.89	0.55
1:C:356:SER:HA	1:C:360:GLY:HA3	1.89	0.55
1:D:180:THR:OG1	1:D:371:LEU:HB2	2.07	0.55
1:H:18:SER:HB3	1:H:23:LEU:HD13	1.89	0.55
1:H:281:VAL:HG23	1:H:475:LEU:HD22	1.89	0.55
1:A:118:PRO:HA	1:A:121:PHE:CZ	2.42	0.55
1:D:281:VAL:HB	1:D:313:ALA:HB3	1.88	0.55
1:G:378:GLN:HB2	1:G:399:TRP:CE3	2.42	0.55
1:A:320:ASN:HD21	1:A:323:TRP:HD1	1.53	0.55
1:B:17:LEU:HD12	1:B:17:LEU:H	1.70	0.55
1:C:177:GLY:HA3	1:C:420:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:VAL:O	1:D:332:THR:OG1	2.21	0.55
1:D:375:GLU:OE2	1:D:405:THR:HG23	2.07	0.55
1:E:122:GLU:HA	1:E:125:ILE:HD11	1.89	0.55
1:F:281:VAL:HG21	1:F:472:ALA:HA	1.89	0.55
1:G:112:ILE:O	1:G:140:LEU:HA	2.07	0.55
1:A:223:PHE:CE2	1:A:310:THR:HG22	2.42	0.54
1:F:198:TRP:HA	1:F:203:ILE:HD12	1.89	0.54
1:G:272:ASN:O	1:G:274:ASP:N	2.33	0.54
1:A:378:GLN:NE2	1:A:401:ASP:OD1	2.40	0.54
1:D:234:GLN:O	1:D:441:GLN:HG2	2.07	0.54
1:E:233:VAL:HG21	1:E:312:VAL:HG11	1.88	0.54
1:H:273:ASN:HB3	1:H:451:GLY:HA2	1.89	0.54
1:B:242:ALA:O	1:B:246:MET:N	2.38	0.54
1:D:141:ALA:HA	1:D:170:TYR:HB2	1.88	0.54
1:D:398:VAL:HG22	1:D:399:TRP:H	1.72	0.54
1:B:336:LEU:HD13	1:B:467:TRP:CE3	2.42	0.54
1:C:173:ASP:OD1	1:C:176:LEU:N	2.31	0.54
1:C:452:TRP:HD1	1:C:453:LYS:N	2.05	0.54
1:E:269:ARG:HB2	1:E:319:ASP:OD2	2.08	0.54
1:E:337:PRO:HD3	1:E:467:TRP:H	1.72	0.54
1:B:413:ARG:HD3	1:B:414:ARG:HH11	1.73	0.54
1:B:228:SER:H	1:B:309:GLU:HG2	1.72	0.54
1:B:281:VAL:HG23	1:B:475:LEU:HD12	1.89	0.54
1:C:251:HIS:NE2	1:D:356:SER:HB2	2.23	0.54
1:F:150:LEU:O	1:F:154:ASP:N	2.30	0.54
1:F:438:VAL:HG12	1:F:442:TRP:CD1	2.42	0.54
1:H:462:TYR:HB2	1:H:466:THR:HG21	1.90	0.54
1:F:437:GLU:O	1:F:441:GLN:N	2.32	0.54
1:G:126:ALA:HA	1:G:163:VAL:HG21	1.88	0.54
1:B:296:ALA:O	1:B:335:ARG:NH2	2.41	0.54
1:C:368:ARG:NH2	2:C:501:HOH:O	2.34	0.54
1:A:213:THR:O	1:A:335:ARG:HA	2.08	0.54
1:F:79:PHE:O	1:F:83:LEU:HD23	2.07	0.54
1:H:175:TYR:CE2	1:H:236:HIS:HB3	2.43	0.54
1:H:298:TYR:O	1:H:302:LEU:N	2.38	0.54
1:A:148:GLN:HG3	1:A:230:ARG:CZ	2.38	0.53
1:A:195:GLU:N	1:A:196:PRO:HD2	2.23	0.53
1:D:150:LEU:HD21	1:D:439:GLU:CG	2.38	0.53
1:E:140:LEU:N	1:E:168:GLN:O	2.39	0.53
1:E:229:LEU:O	1:E:234:GLN:N	2.37	0.53
1:H:117:SER:O	1:H:120:LEU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:VAL:HG12	1:C:311:PHE:HE2	1.74	0.53
1:C:370:VAL:N	1:C:376:THR:O	2.35	0.53
1:D:483:TRP:HA	1:D:483:TRP:HE3	1.74	0.53
1:E:181:VAL:HG22	1:E:371:LEU:HD22	1.89	0.53
1:E:362:LEU:HD13	1:F:190:GLY:HA2	1.90	0.53
1:F:444:TRP:O	1:F:448:ILE:HD13	2.08	0.53
1:H:11:PHE:HD1	1:H:113:TYR:O	1.90	0.53
1:H:363:GLN:HB2	1:H:382:MET:HE3	1.89	0.53
1:B:362:LEU:HG	1:B:395:MET:HE1	1.91	0.53
1:C:343:ILE:HG13	1:C:371:LEU:HD11	1.90	0.53
1:C:404:LEU:HB3	1:C:408:PHE:CE1	2.42	0.53
1:E:340:ARG:NE	1:E:342:GLU:OE2	2.41	0.53
1:H:436:ASP:OD1	1:H:436:ASP:N	2.39	0.53
1:A:320:ASN:HD21	1:A:323:TRP:CD1	2.27	0.53
1:B:213:THR:HG22	1:B:339:ARG:HB2	1.91	0.53
1:C:288:GLY:O	1:C:295:VAL:HG22	2.08	0.53
1:D:142:LEU:N	1:D:170:TYR:O	2.34	0.53
1:D:233:VAL:O	1:D:238:LEU:HB2	2.07	0.53
1:E:258:ARG:HD3	1:E:434:ARG:HD3	1.88	0.53
1:F:173:ASP:CG	1:F:236:HIS:HD1	2.16	0.53
1:F:232:MET:HB3	1:F:237:ILE:HD12	1.90	0.53
1:F:262:VAL:HG11	1:F:436:ASP:HB2	1.90	0.53
1:F:289:VAL:HA	1:F:294:GLU:HA	1.91	0.53
1:G:276:VAL:CG2	1:G:452:TRP:HB3	2.39	0.53
1:H:49:TYR:HB3	1:H:53:GLY:C	2.33	0.53
1:H:50:ASP:H	1:H:53:GLY:HA3	1.74	0.53
1:A:229:LEU:HD12	1:A:312:VAL:HG11	1.90	0.53
1:B:152:SER:O	1:B:153:SER:C	2.51	0.53
1:B:246:MET:HE2	1:B:249:PRO:HD3	1.90	0.53
1:D:284:GLN:HE21	1:D:461:THR:HG22	1.73	0.53
1:G:180:THR:HG21	1:G:375:GLU:HB3	1.90	0.53
1:D:363:GLN:H	1:D:382:MET:HE2	1.72	0.53
1:G:339:ARG:O	1:G:373:PRO:HD3	2.08	0.53
1:H:229:LEU:O	1:H:233:VAL:HB	2.09	0.53
1:E:114:LEU:HB3	1:E:142:LEU:HD23	1.91	0.53
1:F:107:GLU:HA	1:F:137:THR:HG21	1.91	0.53
1:G:21:MET:O	1:G:24:PRO:HD2	2.08	0.53
1:G:165:SER:O	1:G:169:VAL:HG23	2.09	0.53
1:G:377:ILE:HB	1:G:402:LEU:HD23	1.90	0.53
1:G:380:SER:HB3	1:G:399:TRP:CZ2	2.44	0.53
1:A:39:LEU:HD21	1:A:41:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:GLN:NE2	1:C:298:TYR:HB3	2.23	0.53
1:C:419:ARG:HA	1:D:388:LEU:HD11	1.91	0.53
1:F:402:LEU:HA	2:F:502:HOH:O	2.08	0.53
1:C:270:PRO:HA	1:C:444:TRP:CD1	2.44	0.53
1:D:275:THR:HB	1:D:279:HIS:ND1	2.24	0.53
1:E:419:ARG:HD2	1:F:388:LEU:HG	1.90	0.53
1:H:85:TYR:CG	1:H:86:ALA:N	2.76	0.53
1:H:277:ILE:HG23	1:H:278:THR:HG23	1.91	0.53
1:D:346:GLN:HG3	1:D:366:LYS:HG2	1.90	0.52
1:E:390:ARG:O	1:E:394:HIS:CE1	2.63	0.52
1:G:5:VAL:HG22	1:G:110:ILE:N	2.24	0.52
1:G:207:GLN:NE2	1:G:484:TYR:H	2.04	0.52
1:B:94:THR:C	1:B:96:PHE:H	2.16	0.52
1:B:466:THR:O	1:B:467:TRP:HB2	2.09	0.52
1:E:170:TYR:CE2	1:E:429:ALA:HB2	2.44	0.52
1:E:370:VAL:O	1:E:375:GLU:HA	2.08	0.52
1:E:435:ARG:O	1:E:439:GLU:N	2.34	0.52
1:F:296:ALA:O	1:F:335:ARG:NH1	2.42	0.52
1:G:154:ASP:OD1	1:G:435:ARG:NH2	2.42	0.52
1:H:150:LEU:O	1:H:154:ASP:N	2.26	0.52
1:H:215:GLY:HA2	1:H:285:TYR:HE2	1.75	0.52
1:H:230:ARG:CZ	1:H:449:ARG:HD3	2.40	0.52
1:A:383:VAL:HG23	1:B:183:ASN:HB2	1.91	0.52
1:B:381:ILE:HG13	1:B:398:VAL:HG23	1.91	0.52
1:B:437:GLU:O	1:B:441:GLN:N	2.36	0.52
1:E:436:ASP:OD1	1:E:437:GLU:N	2.43	0.52
1:F:486:LEU:HD23	1:F:487:GLU:H	1.74	0.52
1:H:232:MET:O	1:H:237:ILE:HG13	2.09	0.52
1:D:142:LEU:HD11	1:D:169:VAL:HG13	1.91	0.52
1:G:171:ARG:O	1:G:433:VAL:HG23	2.08	0.52
1:H:199:ASN:HA	1:H:322:ARG:HG3	1.90	0.52
1:B:309:GLU:HG2	1:B:309:GLU:O	2.09	0.52
1:C:183:ASN:O	1:C:187:LEU:N	2.35	0.52
1:D:153:SER:O	1:D:157:ASN:N	2.39	0.52
1:D:340:ARG:HH12	1:D:368:ARG:HH22	1.58	0.52
1:G:370:VAL:O	1:G:375:GLU:HA	2.09	0.52
1:F:170:TYR:HB3	1:F:432:PHE:CD1	2.44	0.52
1:G:54:PHE:O	1:G:58:ALA:N	2.40	0.52
1:G:111:ALA:C	1:G:112:ILE:HG12	2.34	0.52
1:G:213:THR:O	1:G:335:ARG:HA	2.10	0.52
1:G:473:ILE:O	1:G:476:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:235:SER:OG	1:H:236:HIS:N	2.43	0.52
1:B:434:ARG:O	1:B:438:VAL:HG23	2.10	0.52
1:B:476:VAL:HG21	1:B:483:TRP:NE1	2.24	0.52
1:C:334:LYS:O	1:C:462:TYR:OH	2.28	0.52
1:E:22:LEU:O	1:E:26:LEU:HD22	2.09	0.52
1:G:140:LEU:HD23	1:G:141:ALA:N	2.24	0.52
1:G:297:GLY:O	1:G:301:GLU:HG3	2.09	0.52
1:A:170:TYR:CE2	1:A:429:ALA:HB3	2.45	0.52
1:B:166:GLU:CD	1:B:171:ARG:HH12	2.17	0.52
1:B:172:ILE:HG12	1:B:432:PHE:HE1	1.75	0.52
1:D:254:ALA:HA	1:D:430:THR:OG1	2.09	0.52
1:F:422:LEU:O	1:F:426:GLU:N	2.33	0.52
1:G:6:SER:O	1:G:39:LEU:HD12	2.10	0.52
1:A:209:SER:HB3	1:A:331:ARG:HE	1.74	0.52
1:B:327:PRO:HB2	1:B:329:TYR:CZ	2.44	0.52
1:D:378:GLN:HB2	1:D:399:TRP:CE3	2.45	0.52
1:G:235:SER:O	1:G:239:GLN:HG2	2.09	0.52
1:A:230:ARG:HG2	1:A:442:TRP:CZ3	2.44	0.52
1:F:112:ILE:HD13	1:F:133:LEU:HD11	1.90	0.52
1:F:315:LYS:HE2	1:F:317:HIS:CE1	2.45	0.52
1:B:188:ARG:HH12	1:B:246:MET:HG2	1.75	0.51
1:E:199:ASN:OD1	1:E:199:ASN:N	2.42	0.51
1:F:438:VAL:HA	1:F:441:GLN:HB2	1.91	0.51
1:G:22:LEU:O	1:G:26:LEU:HD13	2.10	0.51
1:A:400:LEU:HD23	1:B:402:LEU:HB3	1.91	0.51
1:B:197:LEU:O	1:B:202:GLY:HA3	2.09	0.51
1:D:230:ARG:HD2	1:D:442:TRP:CZ3	2.44	0.51
1:G:474:ALA:O	1:G:478:ARG:HG2	2.10	0.51
1:B:198:TRP:HA	1:B:203:ILE:HD11	1.92	0.51
1:E:193:LEU:HA	1:F:197:LEU:HD11	1.93	0.51
1:E:401:ASP:O	1:F:401:ASP:N	2.37	0.51
1:F:378:GLN:HA	1:F:400:LEU:O	2.10	0.51
1:H:233:VAL:HA	1:H:237:ILE:HB	1.92	0.51
1:C:246:MET:HE3	1:C:260:GLU:CB	2.40	0.51
1:D:445:ILE:O	1:D:449:ARG:HG3	2.11	0.51
1:E:154:ASP:OD1	1:E:435:ARG:NH1	2.44	0.51
1:B:357:SER:O	1:B:358:SER:HB2	2.09	0.51
1:E:258:ARG:NH2	1:E:432:PHE:O	2.43	0.51
1:E:335:ARG:CB	1:E:462:TYR:HE1	2.23	0.51
1:F:340:ARG:HH11	1:F:340:ARG:HG2	1.76	0.51
1:G:170:TYR:HB3	1:G:432:PHE:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:THR:HG21	1:H:375:GLU:HG2	1.90	0.51
1:A:252:MET:HG2	1:B:354:ILE:O	2.10	0.51
1:D:312:VAL:HG12	1:D:332:THR:HG22	1.93	0.51
1:E:23:LEU:N	1:E:24:PRO:CD	2.74	0.51
1:A:320:ASN:ND2	1:A:323:TRP:HD1	2.09	0.51
1:C:174:HIS:H	1:C:236:HIS:HE1	1.58	0.51
1:E:362:LEU:HA	1:E:382:MET:SD	2.51	0.51
1:G:195:GLU:N	1:G:196:PRO:HD2	2.26	0.51
1:G:340:ARG:HG3	1:G:373:PRO:CD	2.31	0.51
1:G:452:TRP:O	1:G:456:SER:N	2.43	0.51
1:H:224:ASP:OD2	1:H:302:LEU:HD22	2.11	0.51
1:A:445:ILE:O	1:A:449:ARG:HG3	2.11	0.51
1:D:188:ARG:HH12	1:D:246:MET:HG3	1.75	0.51
1:D:272:ASN:HB2	1:D:275:THR:HG23	1.93	0.51
1:G:262:VAL:HG23	1:G:437:GLU:HG2	1.92	0.51
1:A:269:ARG:HE	1:A:317:HIS:HB2	1.76	0.51
1:D:158:ASP:O	1:D:162:LYS:HB2	2.11	0.51
1:D:276:VAL:HG21	1:D:452:TRP:HB3	1.92	0.51
1:B:335:ARG:HB3	1:B:464:SER:HB3	1.93	0.50
1:B:366:LYS:H	1:B:380:SER:HB2	1.76	0.50
1:C:238:LEU:HD12	1:C:441:GLN:HG2	1.92	0.50
1:A:258:ARG:NH2	1:A:429:ALA:O	2.44	0.50
1:B:10:LEU:C	1:B:11:PHE:HD1	2.18	0.50
1:B:29:LEU:HD21	1:B:32:ASP:HB2	1.93	0.50
1:C:148:GLN:HG2	1:C:230:ARG:NE	2.26	0.50
1:D:281:VAL:HG11	1:D:472:ALA:HB2	1.93	0.50
1:F:466:THR:O	1:F:467:TRP:HB2	2.11	0.50
1:H:165:SER:H	1:H:168:GLN:HG3	1.75	0.50
1:A:24:PRO:O	1:A:25:SER:C	2.53	0.50
1:D:336:LEU:HD22	1:D:467:TRP:HA	1.93	0.50
1:E:133:LEU:HB3	1:E:164:PHE:HE1	1.77	0.50
1:E:390:ARG:O	1:E:394:HIS:HE1	1.93	0.50
1:E:408:PHE:CE1	1:F:385:GLU:HG3	2.46	0.50
1:G:179:GLU:HA	1:G:182:GLN:OE1	2.11	0.50
1:G:225:SER:O	1:G:230:ARG:NH2	2.26	0.50
1:H:30:ASP:HB2	1:H:35:LEU:HD12	1.93	0.50
1:A:184:LEU:HD12	1:A:243:LEU:HD12	1.93	0.50
1:B:185:LEU:HD13	1:B:189:PHE:HD2	1.76	0.50
1:B:333:GLY:HA3	1:B:336:LEU:HD11	1.94	0.50
1:D:170:TYR:HB3	1:D:432:PHE:CD2	2.47	0.50
1:F:96:PHE:CD2	1:F:127:GLY:HA3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:385:GLU:H	1:F:395:MET:HA	1.76	0.50
1:G:141:ALA:HA	1:G:170:TYR:O	2.11	0.50
1:G:357:SER:HB3	1:G:392:GLY:HA2	1.93	0.50
1:H:30:ASP:HA	1:H:35:LEU:HB2	1.93	0.50
1:H:242:ALA:O	1:H:246:MET:HG2	2.11	0.50
1:B:139:ARG:HD3	1:B:170:TYR:HE2	1.76	0.50
1:D:435:ARG:HH21	1:D:436:ASP:HB3	1.76	0.50
1:E:259:ASP:OD1	1:E:434:ARG:NH2	2.43	0.50
1:E:272:ASN:C	1:E:276:VAL:HG23	2.36	0.50
1:E:402:LEU:HD12	1:E:403:SER:N	2.27	0.50
1:F:358:SER:HB3	1:F:392:GLY:HA3	1.92	0.50
1:G:18:SER:HA	1:G:22:LEU:HD12	1.92	0.50
1:A:423:ASP:HB3	1:A:429:ALA:HB1	1.93	0.50
1:C:462:TYR:HD2	1:C:466:THR:HB	1.76	0.50
1:E:386:PRO:HD3	1:F:408:PHE:CE1	2.47	0.50
1:E:449:ARG:HA	1:E:452:TRP:NE1	2.26	0.50
1:F:397:GLU:HG3	1:F:398:VAL:N	2.27	0.50
1:G:207:GLN:HG2	1:G:483:TRP:CZ3	2.47	0.50
1:G:302:LEU:HG	1:G:304:GLN:H	1.76	0.50
1:H:89:ASP:OD1	1:H:90:ILE:N	2.45	0.50
1:A:11:PHE:HA	1:A:44:THR:O	2.12	0.50
1:B:239:GLN:O	1:B:243:LEU:HG	2.12	0.50
1:C:195:GLU:OE1	1:C:322:ARG:NH2	2.31	0.50
1:C:309:GLU:HG3	1:C:311:PHE:O	2.12	0.50
1:C:452:TRP:HB2	1:C:457:MET:CB	2.38	0.50
1:E:187:LEU:HA	1:E:191:ASN:ND2	2.26	0.50
1:H:284:GLN:NE2	1:H:298:TYR:HD2	2.08	0.50
1:D:247:GLU:OE1	1:D:322:ARG:NE	2.40	0.50
1:E:351:PRO:HG3	1:H:201:LYS:HZ1	1.77	0.50
1:F:128:LEU:HD13	1:F:133:LEU:HG	1.92	0.50
1:G:5:VAL:HG22	1:G:109:GLY:CA	2.42	0.50
1:C:404:LEU:HB3	1:C:408:PHE:CD1	2.47	0.49
1:D:215:GLY:C	1:D:217:GLU:H	2.20	0.49
1:E:166:GLU:HA	1:E:169:VAL:CG1	2.35	0.49
1:F:234:GLN:HG3	1:F:442:TRP:CZ3	2.47	0.49
1:B:24:PRO:HB2	1:B:415:ILE:HG13	1.93	0.49
1:B:262:VAL:HG23	1:B:437:GLU:HG2	1.94	0.49
1:E:187:LEU:O	1:E:191:ASN:ND2	2.45	0.49
1:F:56:ASP:HA	1:F:59:GLU:HB3	1.94	0.49
1:F:276:VAL:HG13	1:F:457:MET:HE1	1.93	0.49
1:A:230:ARG:HG2	1:A:442:TRP:HZ3	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LYS:NZ	2:A:506:HOH:O	2.43	0.49
1:F:315:LYS:HE2	1:F:317:HIS:HE1	1.77	0.49
1:A:368:ARG:HB3	1:A:378:GLN:CG	2.43	0.49
1:B:149:ASP:OD1	1:B:152:SER:N	2.38	0.49
1:B:337:PRO:HD3	1:B:467:TRP:HA	1.95	0.49
1:B:413:ARG:NH1	1:B:414:ARG:HD2	2.27	0.49
1:F:128:LEU:O	1:F:131:ALA:HB3	2.11	0.49
1:H:77:ALA:O	1:H:81:ASN:N	2.44	0.49
1:A:121:PHE:O	1:A:125:ILE:HG12	2.12	0.49
1:B:462:TYR:CD1	1:B:469:PRO:HD3	2.47	0.49
1:D:284:GLN:NE2	1:D:461:THR:HG22	2.28	0.49
1:D:309:GLU:CD	1:D:309:GLU:H	2.20	0.49
1:F:486:LEU:O	1:F:487:GLU:HB2	2.11	0.49
1:G:191:ASN:ND2	1:H:382:MET:O	2.46	0.49
1:G:240:LEU:O	1:G:244:VAL:HG23	2.13	0.49
1:H:50:ASP:O	1:H:54:PHE:N	2.40	0.49
1:H:273:ASN:HA	1:H:451:GLY:HA2	1.94	0.49
1:C:297:GLY:O	1:C:301:GLU:HB2	2.13	0.49
1:D:150:LEU:HD21	1:D:439:GLU:HA	1.94	0.49
1:E:173:ASP:OD2	1:E:239:GLN:HG3	2.13	0.49
1:A:199:ASN:O	1:A:201:LYS:N	2.42	0.49
1:B:158:ASP:HA	1:B:161:LEU:HB2	1.94	0.49
1:B:237:ILE:HG21	1:B:330:ILE:HG23	1.93	0.49
1:C:191:ASN:CG	1:D:382:MET:H	2.18	0.49
1:C:309:GLU:O	1:C:309:GLU:HG2	2.10	0.49
1:C:402:LEU:HD21	1:C:404:LEU:HD21	1.95	0.49
1:H:149:ASP:OD1	1:H:152:SER:N	2.35	0.49
1:D:128:LEU:HD23	1:D:133:LEU:HB3	1.94	0.49
1:D:237:ILE:O	1:D:241:VAL:HG23	2.12	0.49
1:D:284:GLN:N	1:D:460:LYS:O	2.45	0.49
1:D:378:GLN:HA	1:D:400:LEU:O	2.13	0.49
1:E:175:TYR:CD2	1:E:236:HIS:HB3	2.48	0.49
1:G:26:LEU:HA	1:G:29:LEU:CD1	2.42	0.49
1:G:99:ILE:O	1:G:100:ALA:HB3	2.13	0.49
1:G:183:ASN:HD21	1:H:383:VAL:HG22	1.78	0.49
1:A:201:LYS:HB3	1:D:201:LYS:HD2	1.95	0.49
1:B:159:ALA:O	1:B:163:VAL:HG23	2.13	0.49
1:E:149:ASP:N	1:E:149:ASP:OD1	2.45	0.49
1:F:258:ARG:NH1	1:F:432:PHE:O	2.45	0.49
1:G:161:LEU:HA	1:G:164:PHE:O	2.12	0.49
1:A:13:SER:N	1:A:45:SER:OG	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:HG2	1:B:323:TRP:CD1	2.48	0.49
1:E:396:ARG:HG2	1:E:396:ARG:HH11	1.78	0.49
1:H:403:SER:O	1:H:407:VAL:HG23	2.13	0.49
1:A:118:PRO:HA	1:A:121:PHE:CE2	2.48	0.48
1:B:185:LEU:HD13	1:B:189:PHE:CD2	2.48	0.48
1:B:476:VAL:HG21	1:B:483:TRP:CD1	2.48	0.48
1:C:197:LEU:HD21	1:D:196:PRO:HG2	1.94	0.48
1:C:411:ARG:CG	1:D:386:PRO:HD2	2.38	0.48
1:D:150:LEU:HD23	1:D:442:TRP:HB2	1.94	0.48
1:D:486:LEU:O	1:D:490:HIS:HB3	2.12	0.48
1:F:48:GLU:HA	1:F:87:THR:HG21	1.95	0.48
1:F:171:ARG:NH2	1:F:434:ARG:HA	2.28	0.48
1:F:209:SER:HA	1:F:331:ARG:O	2.13	0.48
1:G:172:ILE:HG12	1:G:432:PHE:CD1	2.48	0.48
1:E:337:PRO:HD2	1:E:467:TRP:HA	1.94	0.48
1:G:485:ASP:O	1:G:487:GLU:N	2.46	0.48
1:H:236:HIS:HD1	1:H:236:HIS:H	1.61	0.48
1:B:364:PRO:O	1:B:366:LYS:NZ	2.46	0.48
1:C:299:ILE:C	1:C:301:GLU:H	2.20	0.48
1:D:435:ARG:NH2	1:D:436:ASP:HB3	2.28	0.48
1:A:321:TRP:CD1	1:A:321:TRP:C	2.91	0.48
1:A:337:PRO:HD2	1:A:467:TRP:CE3	2.49	0.48
1:B:121:PHE:O	1:B:125:ILE:HG12	2.13	0.48
1:B:442:TRP:O	1:B:446:ASP:N	2.24	0.48
1:C:404:LEU:O	1:C:408:PHE:N	2.44	0.48
1:D:148:GLN:O	1:D:148:GLN:HG2	2.11	0.48
1:E:343:ILE:O	1:E:368:ARG:HA	2.13	0.48
1:F:323:TRP:CZ3	1:F:326:VAL:HG11	2.48	0.48
1:H:195:GLU:N	1:H:196:PRO:HD2	2.29	0.48
1:A:382:MET:HE1	1:A:397:GLU:HB2	1.94	0.48
1:B:379:ILE:O	1:B:399:TRP:HA	2.13	0.48
1:D:421:MET:SD	1:D:421:MET:N	2.86	0.48
1:D:488:HIS:HA	1:D:491:HIS:NE2	2.29	0.48
1:F:48:GLU:HA	1:F:87:THR:CG2	2.44	0.48
1:G:191:ASN:CG	1:H:382:MET:H	2.19	0.48
1:G:378:GLN:HB2	1:G:399:TRP:HE3	1.79	0.48
1:G:412:LYS:CB	1:G:414:ARG:HD2	2.43	0.48
1:H:8:MET:SD	1:H:111:ALA:HB3	2.53	0.48
1:H:271:ILE:HG21	1:H:276:VAL:HG23	1.96	0.48
1:F:10:LEU:HG	1:F:11:PHE:N	2.29	0.48
1:G:41:ILE:O	1:G:83:LEU:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:ASP:HA	1:G:442:TRP:CZ3	2.48	0.48
1:A:147:GLY:O	1:A:442:TRP:CZ2	2.67	0.48
1:B:452:TRP:HB2	1:B:457:MET:HB2	1.95	0.48
1:C:175:TYR:OH	1:C:210:VAL:HG11	2.12	0.48
1:C:194:PHE:HB3	1:C:198:TRP:CZ3	2.49	0.48
1:D:188:ARG:NH1	1:D:246:MET:HG3	2.29	0.48
1:D:309:GLU:HG2	1:D:309:GLU:O	2.13	0.48
1:D:311:PHE:CD1	1:D:336:LEU:HD21	2.49	0.48
1:E:265:PHE:HA	1:E:268:LEU:HD12	1.96	0.48
1:C:369:ILE:HG12	1:C:377:ILE:HG23	1.95	0.48
1:D:141:ALA:HB1	1:D:172:ILE:HD11	1.96	0.48
1:D:385:GLU:HB3	1:D:394:HIS:HB3	1.94	0.48
1:E:408:PHE:CE1	1:F:396:ARG:HD2	2.49	0.48
1:G:18:SER:HA	1:G:22:LEU:HG	1.94	0.48
1:G:143:GLU:HG3	1:G:144:LYS:N	2.29	0.48
1:G:197:LEU:O	1:G:203:ILE:HG13	2.14	0.48
1:G:434:ARG:O	1:G:438:VAL:HG23	2.14	0.48
1:B:47:SER:HB2	1:B:85:TYR:OH	2.14	0.48
1:C:316:ALA:N	1:C:328:PHE:O	2.27	0.48
1:D:195:GLU:OE2	1:D:322:ARG:NH2	2.47	0.48
1:D:197:LEU:O	1:D:202:GLY:HA3	2.14	0.48
1:G:5:VAL:CA	1:G:109:GLY:HA3	2.44	0.48
1:G:11:PHE:HB3	1:G:115:SER:OG	2.14	0.48
1:H:233:VAL:O	1:H:238:LEU:HG	2.14	0.48
1:H:242:ALA:HB1	1:H:261:LYS:HG2	1.95	0.48
1:H:297:GLY:O	1:H:301:GLU:N	2.46	0.48
1:B:99:ILE:O	1:B:102:LEU:HB2	2.14	0.47
1:C:209:SER:O	1:C:341:SER:HA	2.14	0.47
1:C:242:ALA:O	1:C:246:MET:HG2	2.14	0.47
1:D:172:ILE:HG12	1:D:432:PHE:CE2	2.49	0.47
1:E:400:LEU:HA	1:F:402:LEU:HB2	1.95	0.47
1:H:171:ARG:HH12	1:H:435:ARG:HA	1.79	0.47
1:A:283:GLY:HA2	1:A:460:LYS:O	2.14	0.47
1:A:356:SER:HB2	1:B:251:HIS:CE1	2.49	0.47
1:E:259:ASP:O	1:E:262:VAL:HG12	2.14	0.47
1:F:90:ILE:HA	1:F:96:PHE:CZ	2.49	0.47
1:F:288:GLY:HA3	1:F:464:SER:HB2	1.95	0.47
1:F:438:VAL:HG12	1:F:442:TRP:NE1	2.29	0.47
1:G:122:GLU:HG2	1:G:159:ALA:CB	2.44	0.47
1:A:385:GLU:HG3	1:B:408:PHE:CE1	2.49	0.47
1:B:41:ILE:CG2	1:B:83:LEU:HG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.77	0.47
1:B:331:ARG:NH2	1:B:467:TRP:HB3	2.29	0.47
1:C:204:ASP:N	1:C:346:GLN:O	2.41	0.47
1:E:9:ILE:HA	1:E:42:VAL:O	2.15	0.47
1:E:229:LEU:HA	1:E:233:VAL:HB	1.95	0.47
1:E:452:TRP:HA	1:E:455:ASN:HB2	1.97	0.47
1:E:475:LEU:N	2:E:502:HOH:O	2.48	0.47
1:F:315:LYS:HB2	1:F:475:LEU:HD11	1.96	0.47
1:G:439:GLU:O	1:G:443:ILE:HG13	2.14	0.47
1:A:302:LEU:HD23	1:A:304:GLN:H	1.79	0.47
1:B:204:ASP:OD1	1:B:349:PRO:HD3	2.15	0.47
1:B:321:TRP:O	1:C:351:PRO:HB2	2.14	0.47
1:E:143:GLU:HG2	1:E:172:ILE:HB	1.95	0.47
1:F:337:PRO:HG2	1:F:467:TRP:CG	2.49	0.47
1:B:58:ALA:CB	1:B:83:LEU:HD21	2.45	0.47
1:B:92:ASP:C	1:B:94:THR:H	2.22	0.47
1:C:395:MET:HE3	1:C:395:MET:HB2	1.74	0.47
1:D:281:VAL:HG13	1:D:471:THR:HG23	1.96	0.47
1:E:351:PRO:HB2	1:H:321:TRP:O	2.15	0.47
1:F:23:LEU:HD12	1:F:23:LEU:HA	1.73	0.47
1:F:171:ARG:NE	1:F:433:VAL:O	2.47	0.47
1:G:302:LEU:HD21	1:G:304:GLN:HB2	1.96	0.47
1:A:191:ASN:CG	1:B:382:MET:H	2.21	0.47
1:B:322:ARG:HE	1:B:322:ARG:HB2	1.45	0.47
1:F:282:THR:HB	1:F:459:PRO:HA	1.95	0.47
1:G:282:THR:HG21	1:G:309:GLU:HG2	1.96	0.47
1:A:211:ALA:HB3	1:A:340:ARG:H	1.79	0.47
1:A:381:ILE:HD13	1:A:400:LEU:HD11	1.97	0.47
1:D:245:ALA:HB3	1:D:264:VAL:HG13	1.97	0.47
1:D:284:GLN:HE22	1:D:299:ILE:CD1	2.28	0.47
1:D:284:GLN:HE22	1:D:299:ILE:HD11	1.80	0.47
1:D:408:PHE:O	1:D:411:ARG:HB2	2.15	0.47
1:F:54:PHE:CE2	1:F:85:TYR:HB2	2.49	0.47
1:F:150:LEU:HD11	1:F:439:GLU:HG2	1.97	0.47
1:G:288:GLY:HA3	1:G:464:SER:H	1.80	0.47
1:A:180:THR:CG2	1:A:375:GLU:HG2	2.45	0.47
1:A:368:ARG:O	1:A:377:ILE:HA	2.15	0.47
1:B:11:PHE:HB2	1:B:113:TYR:O	2.15	0.47
1:D:366:LYS:H	1:D:380:SER:HB3	1.80	0.47
1:E:185:LEU:N	1:E:185:LEU:HD13	2.29	0.47
1:G:6:SER:OG	1:G:39:LEU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:CYS:HB2	1:G:85:TYR:CD1	2.50	0.47
1:H:11:PHE:O	1:H:115:SER:HB3	2.14	0.47
1:H:452:TRP:HA	1:H:455:ASN:HB2	1.97	0.47
1:A:198:TRP:HA	1:A:203:ILE:HD12	1.97	0.47
1:B:26:LEU:HD13	1:B:26:LEU:C	2.40	0.47
1:B:321:TRP:CE2	1:C:351:PRO:HD2	2.50	0.47
1:G:6:SER:CA	1:G:39:LEU:CD1	2.90	0.47
1:G:18:SER:HA	1:G:22:LEU:CG	2.44	0.47
1:G:337:PRO:HD2	1:G:467:TRP:CD2	2.50	0.47
1:H:50:ASP:C	1:H:53:GLY:H	2.23	0.47
1:B:335:ARG:O	1:B:465:GLY:N	2.48	0.47
1:E:272:ASN:O	1:E:276:VAL:HG23	2.15	0.47
1:F:14:THR:HG22	1:F:45:SER:CB	2.43	0.47
1:F:180:THR:HG21	1:F:371:LEU:O	2.15	0.47
1:G:165:SER:O	1:G:169:VAL:N	2.48	0.47
1:B:253:GLU:O	1:B:257:VAL:HG23	2.15	0.46
1:B:285:TYR:CD1	1:B:335:ARG:HG3	2.50	0.46
1:C:222:TYR:O	1:C:226:SER:N	2.38	0.46
1:C:485:ASP:OD2	1:C:486:LEU:N	2.48	0.46
1:E:200:SER:N	1:E:322:ARG:O	2.48	0.46
1:E:258:ARG:NH2	1:E:429:ALA:O	2.40	0.46
1:G:45:SER:HB3	1:G:85:TYR:OH	2.14	0.46
1:G:114:LEU:HG	1:G:116:THR:CG2	2.45	0.46
1:H:51:THR:HB	1:H:84:PHE:HA	1.96	0.46
1:A:201:LYS:O	1:A:348:LYS:HD2	2.15	0.46
1:A:478:ARG:O	2:A:501:HOH:O	2.20	0.46
1:B:216:LEU:HD22	1:B:334:LYS:HG2	1.97	0.46
1:C:258:ARG:HB3	1:C:434:ARG:NH1	2.31	0.46
1:C:275:THR:O	1:C:279:HIS:HB2	2.16	0.46
1:D:260:GLU:O	1:D:264:VAL:HG23	2.15	0.46
1:E:8:MET:HA	1:E:111:ALA:O	2.15	0.46
1:F:171:ARG:CZ	1:F:434:ARG:HA	2.45	0.46
1:G:357:SER:CB	1:G:392:GLY:HA2	2.45	0.46
1:H:143:GLU:HG3	1:H:417:TYR:OH	2.15	0.46
1:H:151:ALA:O	1:H:155:HIS:HB2	2.15	0.46
1:H:337:PRO:HG2	1:H:467:TRP:CD1	2.49	0.46
1:B:476:VAL:HB	1:B:481:VAL:HB	1.96	0.46
1:C:277:ILE:H	1:C:277:ILE:HG13	1.32	0.46
1:C:311:PHE:CE2	1:C:469:PRO:HD2	2.51	0.46
1:E:128:LEU:HD22	1:E:128:LEU:H	1.80	0.46
1:G:245:ALA:HA	1:G:323:TRP:CZ2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:209:SER:HA	1:H:331:ARG:O	2.15	0.46
1:H:215:GLY:CA	1:H:285:TYR:HE2	2.28	0.46
1:A:90:ILE:HA	1:A:96:PHE:HZ	1.79	0.46
1:A:321:TRP:HA	1:D:352:HIS:HB2	1.96	0.46
1:B:26:LEU:HG	1:B:62:LEU:HA	1.98	0.46
1:B:26:LEU:CD2	1:B:62:LEU:HD12	2.45	0.46
1:B:180:THR:O	1:B:183:ASN:ND2	2.47	0.46
1:B:297:GLY:O	1:B:301:GLU:HG3	2.14	0.46
1:D:449:ARG:HA	1:D:452:TRP:NE1	2.31	0.46
1:E:385:GLU:HG3	1:E:396:ARG:HB2	1.98	0.46
1:F:224:ASP:O	1:F:308:THR:HG21	2.16	0.46
1:F:277:ILE:HG23	1:F:278:THR:HG22	1.96	0.46
1:G:258:ARG:NH1	1:G:429:ALA:O	2.48	0.46
1:A:232:MET:HE2	1:A:232:MET:HB3	1.61	0.46
1:C:144:LYS:HA	1:C:144:LYS:HD2	1.65	0.46
1:H:349:PRO:HD3	1:H:364:PRO:HB3	1.97	0.46
1:B:280:THR:HG22	1:B:314:ILE:HG23	1.98	0.46
1:B:340:ARG:HD2	1:B:368:ARG:NH2	2.31	0.46
1:E:165:SER:H	1:E:168:GLN:HB2	1.80	0.46
1:F:446:ASP:O	1:F:450:GLU:HG3	2.15	0.46
1:F:470:ILE:HA	1:F:473:ILE:HD12	1.97	0.46
1:H:13:SER:OG	1:H:43:CYS:HB3	2.16	0.46
1:H:148:GLN:O	1:H:230:ARG:CZ	2.64	0.46
1:H:434:ARG:NH2	1:H:436:ASP:OD2	2.46	0.46
1:C:239:GLN:O	1:C:243:LEU:HG	2.16	0.46
1:C:282:THR:HB	1:C:459:PRO:HB3	1.98	0.46
1:D:487:GLU:HA	1:D:490:HIS:CD2	2.50	0.46
1:G:204:ASP:OD2	1:G:349:PRO:HD3	2.15	0.46
1:G:271:ILE:HA	1:G:275:THR:HB	1.98	0.46
1:B:385:GLU:OE1	1:B:396:ARG:HB2	2.16	0.46
1:C:245:ALA:HA	1:C:323:TRP:CZ2	2.51	0.46
1:D:311:PHE:HB2	1:D:462:TYR:HE2	1.79	0.46
1:E:10:LEU:HB3	1:E:43:CYS:HA	1.97	0.46
1:E:355:PHE:CZ	1:F:189:PHE:HB2	2.51	0.46
1:G:90:ILE:H	1:G:90:ILE:HG12	1.40	0.46
1:G:378:GLN:HA	1:G:400:LEU:O	2.16	0.46
1:B:378:GLN:HB2	1:B:399:TRP:HE3	1.79	0.46
1:C:188:ARG:NH2	1:C:246:MET:O	2.23	0.46
1:E:283:GLY:N	1:E:311:PHE:HB3	2.20	0.46
1:E:336:LEU:HB3	1:E:467:TRP:CE3	2.51	0.46
1:F:51:THR:HG22	1:F:85:TYR:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:ILE:HG12	1:F:432:PHE:HE1	1.81	0.46
1:G:183:ASN:ND2	1:H:383:VAL:HG22	2.31	0.46
1:B:376:THR:HG23	1:B:402:LEU:O	2.16	0.46
1:C:422:LEU:HD22	1:D:388:LEU:HD22	1.97	0.46
1:D:157:ASN:OD1	1:D:171:ARG:NH2	2.49	0.46
1:F:134:ALA:CB	1:F:163:VAL:HG21	2.45	0.46
1:F:140:LEU:HB3	1:F:168:GLN:O	2.16	0.46
1:G:376:THR:HG23	1:G:402:LEU:O	2.16	0.46
1:H:455:ASN:HB3	1:H:457:MET:HG3	1.98	0.46
1:E:201:LYS:HA	1:E:348:LYS:NZ	2.30	0.45
1:E:202:GLY:CA	1:E:348:LYS:HB2	2.46	0.45
1:E:272:ASN:HB3	1:E:275:THR:HG23	1.98	0.45
1:F:178:LYS:NZ	1:F:178:LYS:HA	2.30	0.45
1:G:43:CYS:HB2	1:G:85:TYR:HD1	1.81	0.45
1:G:216:LEU:HD22	1:G:223:PHE:CD1	2.51	0.45
1:G:258:ARG:HD3	1:G:434:ARG:NH1	2.31	0.45
1:H:142:LEU:CB	1:H:146:LEU:HD11	2.45	0.45
1:H:370:VAL:HG13	1:H:372:GLN:O	2.16	0.45
1:A:474:ALA:O	1:A:478:ARG:HG2	2.15	0.45
1:B:26:LEU:HD22	1:B:26:LEU:O	2.15	0.45
1:B:191:ASN:HB2	1:B:194:PHE:HD2	1.80	0.45
1:B:340:ARG:HD2	1:B:368:ARG:HH21	1.81	0.45
1:C:174:HIS:CD2	1:C:236:HIS:CE1	3.03	0.45
1:C:209:SER:HB2	1:C:331:ARG:HH21	1.82	0.45
1:E:367:LEU:HD12	1:E:378:GLN:O	2.16	0.45
1:H:355:PHE:C	1:H:357:SER:N	2.71	0.45
1:B:281:VAL:HG21	1:B:472:ALA:HA	1.98	0.45
1:B:452:TRP:CD1	1:B:452:TRP:C	2.95	0.45
1:C:226:SER:HB3	1:C:230:ARG:HB2	1.98	0.45
1:C:365:ASN:HA	1:C:380:SER:OG	2.15	0.45
1:F:13:SER:HB3	1:F:44:THR:O	2.15	0.45
1:F:18:SER:O	1:F:23:LEU:HB2	2.16	0.45
1:C:237:ILE:O	1:C:241:VAL:HG23	2.16	0.45
1:E:337:PRO:HD3	1:E:467:TRP:N	2.32	0.45
1:E:358:SER:HB3	1:E:391:ASN:O	2.16	0.45
1:F:213:THR:OG1	1:F:339:ARG:HB2	2.17	0.45
1:H:311:PHE:HB2	1:H:462:TYR:HE2	1.81	0.45
1:B:157:ASN:O	1:B:161:LEU:HG	2.17	0.45
1:B:320:ASN:HD21	1:B:322:ARG:HB3	1.81	0.45
1:D:208:ILE:HG21	1:D:237:ILE:HG23	1.99	0.45
1:G:197:LEU:HD21	1:H:196:PRO:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:269:ARG:O	1:H:444:TRP:NE1	2.44	0.45
1:A:394:HIS:C	1:A:395:MET:HG3	2.42	0.45
1:B:26:LEU:HD23	1:B:62:LEU:HD12	1.97	0.45
1:B:81:ASN:ND2	1:B:81:ASN:H	2.15	0.45
1:D:157:ASN:O	1:D:161:LEU:HB2	2.17	0.45
1:E:8:MET:HG3	1:E:111:ALA:HB3	1.98	0.45
1:F:198:TRP:CD1	1:F:323:TRP:HZ2	2.34	0.45
1:F:285:TYR:CD1	1:F:310:THR:HG21	2.51	0.45
1:G:476:VAL:HB	1:G:481:VAL:O	2.17	0.45
1:A:463:VAL:O	1:A:466:THR:OG1	2.30	0.45
1:B:232:MET:HE3	1:B:232:MET:HB3	1.75	0.45
1:B:251:HIS:HD2	1:B:252:MET:H	1.65	0.45
1:E:272:ASN:O	1:E:276:VAL:N	2.48	0.45
1:G:283:GLY:HA2	1:G:460:LYS:H	1.81	0.45
1:H:49:TYR:O	1:H:85:TYR:CD1	2.70	0.45
1:H:170:TYR:CE2	1:H:424:LEU:HA	2.52	0.45
1:B:102:LEU:HD23	1:B:102:LEU:HA	1.68	0.45
1:B:122:GLU:O	1:B:126:ALA:N	2.49	0.45
1:D:158:ASP:O	1:D:162:LYS:N	2.49	0.45
1:E:274:ASP:OD1	1:E:274:ASP:N	2.49	0.45
1:F:133:LEU:HD22	1:F:133:LEU:HA	1.77	0.45
1:H:230:ARG:NH2	1:H:449:ARG:HD3	2.32	0.45
1:A:273:ASN:HA	1:A:276:VAL:HG12	1.99	0.45
1:B:93:PRO:HA	1:B:96:PHE:CD2	2.52	0.45
1:B:313:ALA:C	1:B:314:ILE:HG13	2.42	0.45
1:C:281:VAL:HG11	1:C:472:ALA:HB2	1.99	0.45
1:C:368:ARG:O	1:C:378:GLN:N	2.38	0.45
1:E:11:PHE:HA	1:E:44:THR:O	2.17	0.45
1:E:331:ARG:CZ	1:E:483:TRP:HB3	2.47	0.45
1:G:93:PRO:HB2	1:G:130:GLN:C	2.41	0.45
1:G:337:PRO:HG3	1:G:465:GLY:HA2	1.98	0.45
1:H:276:VAL:HG11	1:H:451:GLY:C	2.41	0.45
1:B:140:LEU:HB3	1:B:169:VAL:HA	1.99	0.45
1:E:254:ALA:HB2	1:E:428:ASP:CB	2.42	0.45
1:F:60:LYS:HB3	1:F:60:LYS:HE2	1.75	0.45
1:G:143:GLU:HB3	1:G:172:ILE:HB	1.99	0.45
1:H:141:ALA:HB1	1:H:172:ILE:HD11	1.98	0.45
1:B:54:PHE:C	1:B:56:ASP:N	2.76	0.44
1:C:146:LEU:H	1:C:146:LEU:HG	1.48	0.44
1:E:254:ALA:CB	1:E:428:ASP:HB3	2.43	0.44
1:E:351:PRO:HD2	1:H:321:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:LEU:HD23	1:F:185:LEU:HA	1.70	0.44
1:A:11:PHE:O	1:A:45:SER:HA	2.17	0.44
1:A:321:TRP:CD1	1:A:321:TRP:O	2.70	0.44
1:E:195:GLU:N	1:E:196:PRO:HD2	2.32	0.44
1:E:382:MET:HE2	1:E:397:GLU:HA	1.98	0.44
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.84	0.44
1:A:466:THR:O	1:A:467:TRP:HB2	2.16	0.44
1:B:57:PHE:O	1:B:60:LYS:HG3	2.18	0.44
1:B:310:THR:O	1:B:334:LYS:HB2	2.17	0.44
1:C:223:PHE:CZ	1:C:310:THR:HG22	2.51	0.44
1:D:146:LEU:HD23	1:D:171:ARG:NH1	2.33	0.44
1:E:475:LEU:HA	1:E:478:ARG:HB2	1.99	0.44
1:F:246:MET:HE2	1:F:247:GLU:O	2.18	0.44
1:G:246:MET:HA	1:G:264:VAL:HG21	1.99	0.44
1:H:9:ILE:HB	1:H:112:ILE:HG23	1.98	0.44
1:H:262:VAL:HG21	1:H:434:ARG:HH21	1.82	0.44
1:B:195:GLU:N	1:B:196:PRO:HD2	2.33	0.44
1:B:350:VAL:HG21	1:B:362:LEU:HD22	1.99	0.44
1:B:429:ALA:HB3	1:B:432:PHE:HD2	1.83	0.44
1:C:171:ARG:HD2	1:C:433:VAL:HB	1.99	0.44
1:D:170:TYR:CD2	1:D:424:LEU:HD13	2.53	0.44
1:D:408:PHE:HB3	1:D:411:ARG:HG3	2.00	0.44
1:E:140:LEU:HD22	1:E:164:PHE:CE2	2.52	0.44
1:E:232:MET:HE3	1:E:232:MET:HB3	1.92	0.44
1:E:408:PHE:CZ	1:F:385:GLU:HG3	2.53	0.44
1:E:423:ASP:HA	1:E:426:GLU:O	2.17	0.44
1:G:150:LEU:HB2	1:G:442:TRP:HB3	2.00	0.44
1:G:216:LEU:H	1:G:216:LEU:HG	1.54	0.44
1:A:194:PHE:HB3	1:A:198:TRP:CZ3	2.53	0.44
1:A:355:PHE:CZ	1:B:189:PHE:HB2	2.53	0.44
1:A:378:GLN:HG3	1:A:399:TRP:CE3	2.52	0.44
1:B:380:SER:HB3	1:B:397:GLU:CD	2.43	0.44
1:C:210:VAL:HG13	1:C:341:SER:OG	2.18	0.44
1:C:280:THR:HA	1:C:313:ALA:O	2.17	0.44
1:E:153:SER:O	1:E:157:ASN:HB2	2.18	0.44
1:E:362:LEU:CD1	1:F:190:GLY:HA2	2.47	0.44
1:F:9:ILE:HA	1:F:42:VAL:O	2.18	0.44
1:G:6:SER:HB3	1:G:105:PRO:HG2	1.99	0.44
1:G:251:HIS:NE2	1:H:356:SER:HB2	2.33	0.44
1:H:230:ARG:NH1	2:H:502:HOH:O	2.51	0.44
1:A:116:THR:O	1:A:121:PHE:HE1	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ALA:HB2	1:B:297:GLY:H	1.81	0.44
1:C:365:ASN:ND2	1:C:381:ILE:HA	2.32	0.44
1:C:398:VAL:HG22	1:C:399:TRP:H	1.82	0.44
1:E:251:HIS:ND1	1:F:354:ILE:O	2.50	0.44
1:E:287:ALA:HB1	1:E:296:ALA:HB1	1.99	0.44
1:G:452:TRP:HD1	1:G:453:LYS:N	2.16	0.44
1:H:360:GLY:HA2	1:H:395:MET:HE3	2.00	0.44
1:H:370:VAL:O	1:H:375:GLU:HA	2.17	0.44
1:C:368:ARG:N	1:C:378:GLN:O	2.31	0.44
1:D:488:HIS:O	1:D:489:HIS:HB3	2.18	0.44
1:E:151:ALA:O	1:E:155:HIS:HB2	2.17	0.44
1:E:407:VAL:HG21	1:F:398:VAL:HG21	1.99	0.44
1:F:216:LEU:H	1:F:334:LYS:HD2	1.83	0.44
1:F:288:GLY:O	1:F:294:GLU:HG3	2.16	0.44
1:G:337:PRO:HG3	1:G:465:GLY:O	2.18	0.44
1:F:181:VAL:O	1:F:184:LEU:HB2	2.18	0.44
1:G:6:SER:H	1:G:109:GLY:CA	2.28	0.44
1:H:200:SER:N	1:H:322:ARG:O	2.50	0.44
1:A:209:SER:HA	1:A:331:ARG:O	2.18	0.44
1:D:284:GLN:O	1:D:462:TYR:N	2.35	0.44
1:E:107:GLU:H	1:E:107:GLU:HG2	1.37	0.44
1:F:10:LEU:O	1:F:11:PHE:HD1	2.01	0.44
1:G:379:ILE:O	1:G:399:TRP:HA	2.18	0.44
1:A:237:ILE:O	1:A:241:VAL:HG23	2.17	0.43
1:A:265:PHE:HA	1:A:268:LEU:HG	2.00	0.43
1:B:423:ASP:O	1:B:427:GLY:O	2.36	0.43
1:D:258:ARG:HH21	1:D:432:PHE:HB2	1.83	0.43
1:E:475:LEU:HA	1:E:475:LEU:HD23	1.75	0.43
1:F:288:GLY:CA	1:F:464:SER:HB2	2.48	0.43
1:H:271:ILE:CG2	1:H:276:VAL:HG23	2.48	0.43
1:F:172:ILE:HG12	1:F:432:PHE:CE1	2.53	0.43
1:G:18:SER:HA	1:G:22:LEU:CD1	2.47	0.43
1:H:171:ARG:NH1	1:H:435:ARG:HA	2.33	0.43
1:A:318:VAL:HB	1:A:323:TRP:HB2	2.00	0.43
1:B:173:ASP:HB3	1:B:176:LEU:HB2	2.00	0.43
1:C:449:ARG:HA	1:C:452:TRP:NE1	2.33	0.43
1:D:275:THR:O	1:D:279:HIS:HB2	2.18	0.43
1:F:346:GLN:HG3	1:F:366:LYS:HG2	2.00	0.43
1:B:85:TYR:O	1:B:86:ALA:HB3	2.17	0.43
1:C:466:THR:HG22	1:C:466:THR:O	2.18	0.43
1:D:242:ALA:HB1	1:D:261:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:GLN:O	1:E:243:LEU:HG	2.18	0.43
1:E:295:VAL:HG23	1:E:295:VAL:O	2.19	0.43
1:F:60:LYS:HB2	1:F:64:ARG:NH2	2.33	0.43
1:F:396:ARG:NH2	2:F:503:HOH:O	2.51	0.43
1:G:101:ASP:OD1	1:G:101:ASP:N	2.51	0.43
1:G:385:GLU:HG3	1:G:386:PRO:HD2	2.01	0.43
1:B:138:SER:O	1:B:168:GLN:HG2	2.18	0.43
1:B:213:THR:HA	1:B:336:LEU:O	2.19	0.43
1:B:333:GLY:HA3	1:B:336:LEU:CD1	2.48	0.43
1:C:472:ALA:O	1:C:483:TRP:NE1	2.36	0.43
1:D:175:TYR:CD1	1:D:178:LYS:HE2	2.53	0.43
1:D:272:ASN:N	1:D:275:THR:OG1	2.52	0.43
1:E:376:THR:HG22	1:E:402:LEU:O	2.18	0.43
1:E:434:ARG:O	1:E:438:VAL:HG23	2.18	0.43
1:G:7:THR:O	1:G:111:ALA:N	2.49	0.43
1:H:172:ILE:HG12	1:H:432:PHE:CE2	2.52	0.43
1:D:195:GLU:O	1:D:196:PRO:C	2.61	0.43
1:D:242:ALA:HA	1:D:264:VAL:HG11	2.01	0.43
1:E:272:ASN:N	1:E:275:THR:OG1	2.43	0.43
1:F:210:VAL:HG21	1:F:237:ILE:HG12	2.01	0.43
1:F:213:THR:HG23	1:F:339:ARG:N	2.33	0.43
1:H:180:THR:CG2	1:H:375:GLU:HG2	2.48	0.43
1:A:180:THR:HG22	1:A:375:GLU:HG2	2.00	0.43
1:A:289:VAL:HA	1:A:294:GLU:HA	2.01	0.43
1:A:378:GLN:HG3	1:A:399:TRP:CZ3	2.53	0.43
1:B:41:ILE:HG21	1:B:83:LEU:HG	2.01	0.43
1:C:270:PRO:HA	1:C:444:TRP:HD1	1.82	0.43
1:D:171:ARG:NE	1:D:438:VAL:HG11	2.32	0.43
1:D:362:LEU:HA	1:D:382:MET:HE2	2.00	0.43
1:F:385:GLU:OE2	1:F:396:ARG:HB2	2.17	0.43
1:G:157:ASN:O	1:G:161:LEU:HG	2.19	0.43
1:G:358:SER:N	1:G:392:GLY:HA3	2.34	0.43
1:G:368:ARG:HG2	1:G:378:GLN:HE21	1.84	0.43
1:H:8:MET:HA	1:H:111:ALA:O	2.17	0.43
1:H:112:ILE:N	1:H:139:ARG:O	2.51	0.43
1:H:246:MET:HE3	1:H:260:GLU:HB3	2.01	0.43
1:A:136:PRO:O	1:A:137:THR:C	2.60	0.43
1:A:211:ALA:HB1	1:A:338:ALA:O	2.18	0.43
1:A:379:ILE:HD11	1:B:400:LEU:HD13	2.00	0.43
1:E:355:PHE:C	1:E:357:SER:H	2.26	0.43
1:F:177:GLY:O	1:F:416:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:SER:O	1:H:87:THR:HA	2.19	0.43
1:H:171:ARG:O	1:H:433:VAL:HG23	2.19	0.43
1:H:423:ASP:O	1:H:426:GLU:O	2.35	0.43
1:B:51:THR:OG1	1:B:52:ASP:N	2.51	0.43
1:C:316:ALA:HB3	1:C:328:PHE:HB2	2.00	0.43
1:D:415:ILE:O	1:D:418:GLU:HG3	2.19	0.43
1:F:302:LEU:HD12	2:F:506:HOH:O	2.19	0.43
1:G:146:LEU:HD11	1:G:234:GLN:CD	2.44	0.43
1:A:419:ARG:HD3	1:B:388:LEU:HD23	2.00	0.43
1:B:331:ARG:HH21	1:B:467:TRP:HB3	1.84	0.43
1:B:449:ARG:O	1:B:452:TRP:CD1	2.72	0.43
1:C:176:LEU:HD21	1:C:239:GLN:HB3	2.01	0.43
1:D:403:SER:O	1:D:407:VAL:HG23	2.18	0.43
1:F:139:ARG:HG2	2:F:519:HOH:O	2.19	0.43
1:G:23:LEU:N	1:G:24:PRO:CD	2.82	0.43
1:G:251:HIS:CG	1:G:252:MET:H	2.37	0.43
1:H:299:ILE:HD12	1:H:306:SER:H	1.83	0.43
1:A:444:TRP:O	1:A:448:ILE:HG13	2.18	0.42
1:B:347:PHE:HB2	1:B:365:ASN:O	2.18	0.42
1:C:195:GLU:N	1:C:196:PRO:HD2	2.33	0.42
1:G:5:VAL:CG1	1:G:111:ALA:HB2	2.44	0.42
1:G:175:TYR:OH	1:G:232:MET:HE1	2.19	0.42
1:H:234:GLN:HG3	1:H:445:ILE:HG13	2.01	0.42
1:H:323:TRP:HZ3	1:H:326:VAL:HG11	1.84	0.42
1:H:329:TYR:OH	1:H:479:ASP:OD2	2.34	0.42
1:H:452:TRP:HB2	1:H:457:MET:HB2	2.00	0.42
1:A:45:SER:HB2	1:A:85:TYR:HE1	1.84	0.42
1:B:354:ILE:H	1:B:354:ILE:HG12	1.45	0.42
1:B:399:TRP:CZ2	1:B:484:TYR:HE2	2.37	0.42
1:C:166:GLU:OE2	1:C:435:ARG:HB2	2.19	0.42
1:D:173:ASP:HB3	1:D:176:LEU:HD12	2.00	0.42
1:D:239:GLN:NE2	1:D:433:VAL:HG13	2.34	0.42
1:E:81:ASN:OD1	1:E:81:ASN:N	2.51	0.42
1:F:378:GLN:HB3	1:F:401:ASP:HA	2.01	0.42
1:G:276:VAL:HG23	1:G:280:THR:OG1	2.19	0.42
1:G:419:ARG:NH2	1:H:389:ASP:HB2	2.34	0.42
1:H:172:ILE:HG23	1:H:420:LEU:HD22	2.01	0.42
1:H:385:GLU:N	1:H:395:MET:HA	2.32	0.42
1:B:347:PHE:N	1:B:365:ASN:O	2.51	0.42
1:D:140:LEU:HD11	1:D:142:LEU:HG	2.01	0.42
1:E:40:ARG:HA	1:E:82:LYS:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:TYR:CE2	1:E:236:HIS:HB3	2.53	0.42
1:E:202:GLY:C	1:E:348:LYS:HB2	2.44	0.42
1:E:277:ILE:HD12	1:E:277:ILE:HA	1.83	0.42
1:F:43:CYS:N	1:F:84:PHE:O	2.41	0.42
1:H:8:MET:SD	1:H:111:ALA:O	2.77	0.42
1:A:318:VAL:HB	1:A:323:TRP:CB	2.48	0.42
1:B:157:ASN:O	1:B:161:LEU:N	2.41	0.42
1:C:153:SER:O	1:C:157:ASN:HB2	2.19	0.42
1:F:150:LEU:O	1:F:151:ALA:C	2.62	0.42
1:G:395:MET:SD	1:H:186:THR:HG23	2.60	0.42
1:G:419:ARG:HH21	1:G:423:ASP:CG	2.27	0.42
1:H:234:GLN:CG	1:H:445:ILE:HG13	2.49	0.42
1:A:340:ARG:HG2	1:A:373:PRO:HD3	2.02	0.42
1:B:181:VAL:HA	1:B:184:LEU:HG	2.00	0.42
1:C:308:THR:N	2:C:506:HOH:O	2.53	0.42
1:D:204:ASP:O	1:D:326:VAL:HG13	2.19	0.42
1:D:335:ARG:O	1:D:462:TYR:HE1	2.02	0.42
1:E:199:ASN:OD1	1:E:201:LYS:O	2.36	0.42
1:F:114:LEU:HB2	1:F:142:LEU:HD23	2.01	0.42
1:F:198:TRP:CD1	1:F:323:TRP:CZ2	3.08	0.42
1:F:238:LEU:HD23	1:F:238:LEU:HA	1.64	0.42
1:H:35:LEU:HD23	1:H:35:LEU:HA	1.90	0.42
1:H:150:LEU:O	1:H:154:ASP:HB2	2.18	0.42
1:D:254:ALA:HB1	1:D:429:ALA:O	2.19	0.42
1:E:125:ILE:HA	1:E:128:LEU:HD23	2.02	0.42
1:F:128:LEU:CD1	1:F:133:LEU:HG	2.49	0.42
1:F:147:GLY:O	1:F:442:TRP:CH2	2.72	0.42
1:F:311:PHE:CD2	1:F:333:GLY:HA3	2.54	0.42
1:A:237:ILE:HG21	1:A:330:ILE:CG2	2.50	0.42
1:B:23:LEU:HD22	1:B:23:LEU:HA	1.77	0.42
1:B:268:LEU:HD22	1:B:444:TRP:CZ2	2.54	0.42
1:B:337:PRO:HD3	1:B:467:TRP:N	2.35	0.42
1:C:264:VAL:O	1:C:267:ALA:N	2.51	0.42
1:D:150:LEU:CD2	1:D:439:GLU:HA	2.50	0.42
1:D:275:THR:HB	1:D:279:HIS:HD1	1.84	0.42
1:E:80:LEU:HD13	1:E:80:LEU:HA	1.75	0.42
1:E:171:ARG:HB2	1:E:433:VAL:O	2.20	0.42
1:E:392:GLY:O	1:E:394:HIS:CE1	2.72	0.42
1:F:85:TYR:CD2	1:F:86:ALA:N	2.87	0.42
1:F:302:LEU:HG	1:F:304:GLN:H	1.85	0.42
1:F:403:SER:N	2:F:502:HOH:O	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:ARG:HA	1:F:452:TRP:NE1	2.34	0.42
1:G:169:VAL:O	1:G:170:TYR:HD1	2.02	0.42
1:G:404:LEU:HD22	1:G:408:PHE:HE2	1.85	0.42
1:H:417:TYR:O	1:H:421:MET:HE2	2.20	0.42
1:A:475:LEU:HD12	1:A:478:ARG:HH21	1.84	0.42
1:B:211:ALA:HB1	1:B:338:ALA:O	2.20	0.42
1:B:307:ASP:O	1:B:459:PRO:HG3	2.19	0.42
1:B:476:VAL:HG21	1:B:483:TRP:HE1	1.83	0.42
1:D:379:ILE:HB	1:D:400:LEU:HD12	2.02	0.42
1:E:284:GLN:HA	1:E:310:THR:OG1	2.20	0.42
1:E:342:GLU:HA	1:E:369:ILE:O	2.20	0.42
1:F:72:ASN:HB2	1:F:75:ALA:HB3	2.01	0.42
1:H:176:LEU:HA	1:H:176:LEU:HD23	1.77	0.42
1:A:99:ILE:H	1:A:99:ILE:HG12	1.36	0.42
1:B:26:LEU:HD21	1:B:30:ASP:HB3	2.02	0.42
1:B:161:LEU:HA	1:B:164:PHE:O	2.19	0.42
1:B:245:ALA:HA	1:B:323:TRP:HE1	1.85	0.42
1:C:154:ASP:HA	1:C:435:ARG:NH2	2.30	0.42
1:C:414:ARG:NH2	2:C:505:HOH:O	2.52	0.42
1:E:178:LYS:HB2	1:E:181:VAL:CG2	2.48	0.42
1:G:226:SER:OG	1:G:230:ARG:HB2	2.20	0.42
1:G:438:VAL:HG12	1:G:442:TRP:HD1	1.85	0.42
1:H:285:TYR:CB	1:H:298:TYR:HB2	2.37	0.42
1:A:164:PHE:HB3	1:A:168:GLN:HB2	2.01	0.42
1:B:485:ASP:OD1	1:B:486:LEU:N	2.52	0.42
1:C:279:HIS:HA	1:C:475:LEU:HD11	2.02	0.42
1:D:180:THR:HG21	1:D:375:GLU:HG2	2.00	0.42
1:G:146:LEU:HD11	1:G:234:GLN:OE1	2.20	0.42
1:G:463:VAL:HB	1:G:466:THR:HG23	2.01	0.42
1:D:232:MET:O	1:D:236:HIS:HB2	2.20	0.41
1:D:246:MET:HE3	1:D:260:GLU:HB2	2.02	0.41
1:E:139:ARG:HA	1:E:168:GLN:CA	2.46	0.41
1:E:171:ARG:HB3	1:E:433:VAL:HB	2.03	0.41
1:E:388:LEU:HD13	1:F:419:ARG:HA	2.01	0.41
1:E:478:ARG:HD2	1:E:478:ARG:HA	1.77	0.41
1:F:21:MET:O	1:F:24:PRO:HG2	2.19	0.41
1:F:118:PRO:O	1:F:119:SER:HB2	2.20	0.41
1:F:423:ASP:HB3	1:F:429:ALA:CB	2.49	0.41
1:G:295:VAL:HB	1:G:335:ARG:HH12	1.85	0.41
1:C:253:GLU:O	1:C:257:VAL:HG23	2.20	0.41
1:G:484:TYR:CE2	1:G:486:LEU:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:335:ARG:O	1:H:462:TYR:HE1	2.03	0.41
1:H:383:VAL:HB	1:H:398:VAL:HG11	2.02	0.41
1:A:395:MET:HE3	1:A:395:MET:HB2	1.98	0.41
1:B:382:MET:HG2	1:B:395:MET:HE2	2.02	0.41
1:C:404:LEU:CD2	1:D:383:VAL:HG21	2.51	0.41
1:D:142:LEU:HD12	1:D:170:TYR:O	2.20	0.41
1:E:383:VAL:HG21	1:F:404:LEU:HD22	2.01	0.41
1:F:215:GLY:HA2	1:F:334:LYS:CD	2.49	0.41
1:G:38:ASP:OD1	1:G:38:ASP:N	2.53	0.41
1:H:41:ILE:HB	1:H:83:LEU:HD23	2.02	0.41
1:H:150:LEU:HD11	1:H:439:GLU:HG3	2.01	0.41
1:H:337:PRO:HG3	1:H:465:GLY:C	2.45	0.41
1:A:419:ARG:HD3	1:B:388:LEU:HB3	2.02	0.41
1:B:320:ASN:ND2	1:B:322:ARG:H	2.19	0.41
1:B:354:ILE:HD11	1:C:321:TRP:CE3	2.56	0.41
1:C:207:GLN:HB2	1:C:344:VAL:HB	2.02	0.41
1:C:368:ARG:HB3	1:C:399:TRP:HZ3	1.85	0.41
1:D:448:ILE:HG22	1:D:452:TRP:HD1	1.85	0.41
1:F:210:VAL:HB	1:F:332:THR:HB	2.03	0.41
1:F:229:LEU:HD12	1:F:312:VAL:HG21	2.02	0.41
1:G:43:CYS:HB3	1:G:54:PHE:CE2	2.55	0.41
1:G:161:LEU:HD22	1:G:165:SER:HA	2.03	0.41
1:H:118:PRO:O	1:H:119:SER:OG	2.29	0.41
1:H:238:LEU:HA	1:H:238:LEU:HD23	1.75	0.41
1:A:201:LYS:H	1:A:201:LYS:HG2	1.68	0.41
1:B:411:ARG:HA	1:B:411:ARG:HD3	1.85	0.41
1:E:287:ALA:CB	1:E:296:ALA:HB1	2.50	0.41
1:G:288:GLY:HA3	1:G:463:VAL:HG13	2.02	0.41
1:G:337:PRO:HD2	1:G:467:TRP:CG	2.56	0.41
1:G:452:TRP:HB2	1:G:457:MET:HG3	2.03	0.41
1:H:371:LEU:H	1:H:371:LEU:HG	1.70	0.41
1:A:149:ASP:HB2	1:A:152:SER:OG	2.21	0.41
1:E:272:ASN:OD1	1:E:273:ASN:N	2.54	0.41
1:E:414:ARG:HA	1:E:414:ARG:HD2	1.97	0.41
1:F:232:MET:O	1:F:236:HIS:HB2	2.20	0.41
1:G:173:ASP:OD2	1:G:235:SER:HB2	2.20	0.41
1:G:457:MET:HB3	1:G:457:MET:HE2	1.70	0.41
1:H:212:GLU:HB2	1:H:333:GLY:O	2.21	0.41
1:A:321:TRP:HA	1:D:352:HIS:CB	2.50	0.41
1:A:368:ARG:HB3	1:A:378:GLN:HG2	2.02	0.41
1:A:384:LYS:H	1:B:183:ASN:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ILE:HG23	1:B:42:VAL:HG11	2.02	0.41
1:B:26:LEU:CD2	1:B:30:ASP:HB3	2.50	0.41
1:B:172:ILE:HG12	1:B:432:PHE:CE1	2.55	0.41
1:C:187:LEU:HD13	1:C:377:ILE:HD13	2.03	0.41
1:C:452:TRP:CD1	1:C:453:LYS:N	2.88	0.41
1:D:487:GLU:HA	1:D:490:HIS:NE2	2.35	0.41
1:E:166:GLU:CA	1:E:169:VAL:HG12	2.43	0.41
1:F:17:LEU:HD22	1:F:17:LEU:HA	1.75	0.41
1:F:154:ASP:O	1:F:158:ASP:N	2.43	0.41
1:G:368:ARG:HB3	1:G:378:GLN:HG3	2.03	0.41
1:H:285:TYR:N	1:H:310:THR:OG1	2.54	0.41
1:A:242:ALA:HB2	1:A:265:PHE:CZ	2.56	0.41
1:C:433:VAL:HG12	1:C:437:GLU:HB2	2.01	0.41
1:D:311:PHE:CD1	1:D:333:GLY:HA3	2.56	0.41
1:F:343:ILE:O	1:F:368:ARG:HA	2.20	0.41
1:F:358:SER:CB	1:F:392:GLY:HA3	2.50	0.41
1:G:183:ASN:HD21	1:H:383:VAL:CG2	2.33	0.41
1:G:423:ASP:HB2	1:G:432:PHE:HE2	1.85	0.41
1:G:452:TRP:CD1	1:G:452:TRP:C	2.96	0.41
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.82	0.41
1:A:189:PHE:CE1	1:A:248:PRO:HB3	2.56	0.41
1:A:322:ARG:HG2	1:A:323:TRP:CD1	2.56	0.41
1:A:355:PHE:CD2	1:B:252:MET:HG3	2.56	0.41
1:A:452:TRP:CD1	1:A:452:TRP:C	2.99	0.41
1:B:133:LEU:HD23	1:B:133:LEU:HA	1.83	0.41
1:B:200:SER:HA	1:B:326:VAL:HG21	2.03	0.41
1:B:251:HIS:CD2	1:B:252:MET:H	2.39	0.41
1:B:259:ASP:OD1	1:B:434:ARG:NH1	2.44	0.41
1:B:422:LEU:HD23	1:B:423:ASP:N	2.36	0.41
1:C:238:LEU:HD23	1:C:238:LEU:HA	1.91	0.41
1:C:340:ARG:HA	1:C:373:PRO:HD3	2.03	0.41
1:D:150:LEU:HD23	1:D:150:LEU:HA	1.84	0.41
1:D:245:ALA:HA	1:D:323:TRP:NE1	2.36	0.41
1:D:302:LEU:HD23	1:D:302:LEU:HA	1.86	0.41
1:D:488:HIS:H	1:D:488:HIS:CD2	2.38	0.41
1:E:40:ARG:CB	1:E:84:PHE:HE2	2.34	0.41
1:E:164:PHE:HA	1:E:168:GLN:OE1	2.21	0.41
1:E:212:GLU:HB3	1:E:214:VAL:HG22	2.02	0.41
1:E:230:ARG:CZ	1:E:449:ARG:HD3	2.51	0.41
1:E:452:TRP:CD1	1:E:452:TRP:C	2.99	0.41
1:F:41:ILE:HG22	1:F:43:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:ASP:C	1:F:59:GLU:H	2.28	0.41
1:F:60:LYS:H	1:F:60:LYS:HG2	1.36	0.41
1:F:434:ARG:NE	1:F:436:ASP:OD2	2.54	0.41
1:G:114:LEU:HA	1:G:114:LEU:HD12	1.81	0.41
1:H:37:ASP:OD1	1:H:37:ASP:N	2.52	0.41
1:H:273:ASN:CA	1:H:451:GLY:HA2	2.50	0.41
1:H:433:VAL:HG12	1:H:437:GLU:HB2	2.03	0.41
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.77	0.41
1:B:50:ASP:OD2	1:B:50:ASP:N	2.53	0.41
1:B:180:THR:HA	1:B:183:ASN:HD22	1.86	0.41
1:B:333:GLY:HA3	1:B:336:LEU:HG	2.03	0.41
1:E:176:LEU:HA	1:E:176:LEU:HD12	1.89	0.41
1:E:477:GLU:C	1:E:480:GLY:H	2.28	0.41
1:F:41:ILE:O	1:F:84:PHE:N	2.51	0.41
1:F:83:LEU:HA	1:F:83:LEU:HD22	1.86	0.41
1:F:133:LEU:HD13	1:F:138:SER:HB3	2.02	0.41
1:F:173:ASP:OD2	1:F:235:SER:HB2	2.21	0.41
1:F:408:PHE:HD1	1:F:411:ARG:HD3	1.85	0.41
1:G:446:ASP:O	1:G:450:GLU:HB2	2.20	0.41
1:H:223:PHE:CE1	1:H:310:THR:HG22	2.56	0.41
1:B:10:LEU:HG	1:B:11:PHE:N	2.34	0.40
1:B:213:THR:HG22	1:B:339:ARG:CB	2.51	0.40
1:C:357:SER:OG	1:C:358:SER:N	2.54	0.40
1:F:167:LYS:H	1:F:167:LYS:HG3	1.68	0.40
1:F:171:ARG:O	1:F:433:VAL:HG23	2.22	0.40
1:G:5:VAL:HG11	1:G:111:ALA:CB	2.45	0.40
1:G:227:GLY:O	1:G:231:ASP:HB2	2.21	0.40
1:H:146:LEU:HB3	1:H:156:ILE:HD11	2.03	0.40
1:H:316:ALA:N	1:H:328:PHE:O	2.53	0.40
1:A:162:LYS:H	1:A:162:LYS:HG2	1.45	0.40
1:A:462:TYR:CD1	1:A:469:PRO:HD3	2.56	0.40
1:C:183:ASN:ND2	1:D:383:VAL:HG23	2.35	0.40
1:C:288:GLY:H	1:C:295:VAL:HG22	1.86	0.40
1:D:126:ALA:O	1:D:130:GLN:HB2	2.21	0.40
1:E:128:LEU:HD12	1:E:133:LEU:HD13	2.03	0.40
1:F:64:ARG:HA	1:F:64:ARG:HD3	1.49	0.40
1:G:130:GLN:HE21	1:G:130:GLN:HB2	1.58	0.40
1:G:209:SER:HB2	1:G:483:TRP:CZ3	2.56	0.40
1:G:299:ILE:HD13	1:G:299:ILE:HA	1.76	0.40
1:H:8:MET:CE	1:H:424:LEU:HD21	2.51	0.40
1:A:368:ARG:HB3	1:A:378:GLN:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ILE:O	1:A:399:TRP:HA	2.22	0.40
1:B:54:PHE:C	1:B:56:ASP:H	2.29	0.40
1:B:348:LYS:HA	1:B:349:PRO:HD3	1.89	0.40
1:C:230:ARG:O	1:C:234:GLN:HB3	2.21	0.40
1:D:285:TYR:HB2	1:D:310:THR:HG21	2.03	0.40
1:E:7:THR:HB	1:E:110:ILE:CB	2.52	0.40
1:E:142:LEU:HB3	1:E:146:LEU:HD21	2.04	0.40
1:E:352:HIS:HB3	1:H:321:TRP:HA	2.04	0.40
1:F:26:LEU:HB3	1:F:79:PHE:CE1	2.56	0.40
1:F:118:PRO:HA	1:F:121:PHE:HE2	1.86	0.40
1:G:299:ILE:O	1:G:303:GLY:N	2.43	0.40
1:H:51:THR:HA	1:H:85:TYR:H	1.86	0.40
1:H:89:ASP:OD1	1:H:91:THR:OG1	2.39	0.40
1:H:344:VAL:HG21	1:H:484:TYR:CD2	2.57	0.40
1:H:345:VAL:O	1:H:366:LYS:HA	2.22	0.40
1:B:370:VAL:HG23	1:B:376:THR:HB	2.04	0.40
1:F:139:ARG:NH1	1:F:424:LEU:O	2.55	0.40
1:G:16:ASP:OD2	1:G:17:LEU:HG	2.21	0.40
1:G:357:SER:OG	1:G:392:GLY:HA2	2.21	0.40
1:G:405:THR:O	1:G:409:LYS:HA	2.22	0.40
1:A:363:GLN:N	1:A:382:MET:HE2	2.16	0.40
1:A:385:GLU:HG3	1:B:408:PHE:HE1	1.85	0.40
1:B:58:ALA:HB2	1:B:83:LEU:HD21	2.02	0.40
1:D:239:GLN:HE22	1:D:433:VAL:HG13	1.86	0.40
1:D:442:TRP:HA	1:D:445:ILE:HB	2.03	0.40
1:E:484:TYR:CZ	1:E:486:LEU:O	2.75	0.40
1:F:157:ASN:HB2	1:F:435:ARG:HH21	1.85	0.40
1:F:200:SER:N	1:F:322:ARG:O	2.53	0.40
1:G:34:LEU:HD22	1:G:34:LEU:HA	1.75	0.40
1:G:271:ILE:HG23	1:G:275:THR:HB	2.03	0.40
1:G:282:THR:HB	1:G:309:GLU:HB3	2.04	0.40
1:G:380:SER:HB3	1:G:399:TRP:CE2	2.57	0.40
1:H:271:ILE:HB	1:H:448:ILE:HG12	2.02	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	447/493 (91%)	415 (93%)	32 (7%)	0	100	100
1	B	455/493 (92%)	425 (93%)	30 (7%)	0	100	100
1	C	341/493 (69%)	310 (91%)	31 (9%)	0	100	100
1	D	357/493 (72%)	327 (92%)	30 (8%)	0	100	100
1	E	440/493 (89%)	396 (90%)	44 (10%)	0	100	100
1	F	478/493 (97%)	440 (92%)	38 (8%)	0	100	100
1	G	459/493 (93%)	421 (92%)	38 (8%)	0	100	100
1	H	470/493 (95%)	431 (92%)	39 (8%)	0	100	100
All	All	3447/3944 (87%)	3165 (92%)	282 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	330/417 (79%)	265 (80%)	65 (20%)	1	4
1	B	366/417 (88%)	286 (78%)	80 (22%)	1	3
1	C	280/417 (67%)	241 (86%)	39 (14%)	3	11
1	D	278/417 (67%)	241 (87%)	37 (13%)	4	12
1	E	336/417 (81%)	270 (80%)	66 (20%)	1	4
1	F	370/417 (89%)	301 (81%)	69 (19%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	361/417 (87%)	294 (81%)	67 (19%)	1	5
1	H	348/417 (84%)	302 (87%)	46 (13%)	4	12
All	All	2669/3336 (80%)	2200 (82%)	469 (18%)	2	6

All (469) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	17	LEU
1	A	18	SER
1	A	23	LEU
1	A	25	SER
1	A	27	TYR
1	A	30	ASP
1	A	38	ASP
1	A	39	LEU
1	A	80	LEU
1	A	83	LEU
1	A	91	THR
1	A	94	THR
1	A	99	ILE
1	A	106	VAL
1	A	116	THR
1	A	117	SER
1	A	128	LEU
1	A	133	LEU
1	A	140	LEU
1	A	143	GLU
1	A	146	LEU
1	A	148	GLN
1	A	150	LEU
1	A	168	GLN
1	A	169	VAL
1	A	174	HIS
1	A	179	GLU
1	A	193	LEU
1	A	204	ASP
1	A	212	GLU
1	A	224	ASP
1	A	226	SER
1	A	228	SER

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Mol	Chain	Res	Type
1	A	232	MET
1	A	236	HIS
1	A	237	ILE
1	A	257	VAL
1	A	277	ILE
1	A	278	THR
1	A	281	VAL
1	A	282	THR
1	A	289	VAL
1	A	302	LEU
1	A	321	TRP
1	A	322	ARG
1	A	330	ILE
1	A	346	GLN
1	A	354	ILE
1	A	357	SER
1	A	366	LYS
1	A	371	LEU
1	A	380	SER
1	A	383	VAL
1	A	401	ASP
1	A	403	SER
1	A	419	ARG
1	A	421	MET
1	A	433	VAL
1	A	434	ARG
1	A	436	ASP
1	A	450	GLU
1	A	461	THR
1	A	485	ASP
1	A	486	LEU
1	B	10	LEU
1	B	13	SER
1	B	14	THR
1	B	16	ASP
1	B	17	LEU
1	B	18	SER
1	B	21	MET
1	B	23	LEU
1	B	26	LEU
1	B	27	TYR
1	B	30	ASP

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Mol	Chain	Res	Type
1	B	34	LEU
1	B	37	ASP
1	B	38	ASP
1	B	39	LEU
1	B	43	CYS
1	B	44	THR
1	B	45	SER
1	B	46	ARG
1	B	50	ASP
1	B	80	LEU
1	B	81	ASN
1	B	83	LEU
1	B	88	VAL
1	B	102	LEU
1	B	106	VAL
1	B	114	LEU
1	B	116	THR
1	B	119	SER
1	B	122	GLU
1	B	128	LEU
1	B	146	LEU
1	B	149	ASP
1	B	150	LEU
1	B	152	SER
1	B	155	HIS
1	B	160	VAL
1	B	162	LYS
1	B	163	VAL
1	B	183	ASN
1	B	199	ASN
1	B	201	LYS
1	B	213	THR
1	B	216	LEU
1	B	220	ILE
1	B	225	SER
1	B	226	SER
1	B	228	SER
1	B	236	HIS
1	B	237	ILE
1	B	262	VAL
1	B	266	ARG
1	B	268	LEU

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Mol	Chain	Res	Type
1	B	277	ILE
1	B	289	VAL
1	B	290	SER
1	B	307	ASP
1	B	312	VAL
1	B	314	ILE
1	B	320	ASN
1	B	322	ARG
1	B	331	ARG
1	B	334	LYS
1	B	340	ARG
1	B	344	VAL
1	B	348	LYS
1	B	354	ILE
1	B	356	SER
1	B	370	VAL
1	B	378	GLN
1	B	388	LEU
1	B	402	LEU
1	B	405	THR
1	B	410	ASP
1	B	422	LEU
1	B	426	GLU
1	B	428	ASP
1	B	433	VAL
1	B	436	ASP
1	B	464	SER
1	C	140	LEU
1	C	142	LEU
1	C	144	LYS
1	C	146	LEU
1	C	155	HIS
1	C	161	LEU
1	C	163	VAL
1	C	172	ILE
1	C	174	HIS
1	C	176	LEU
1	C	220	ILE
1	C	235	SER
1	C	238	LEU
1	C	253	GLU
1	C	274	ASP

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Mol	Chain	Res	Type
1	C	277	ILE
1	C	278	THR
1	C	280	THR
1	C	282	THR
1	C	302	LEU
1	C	307	ASP
1	C	308	THR
1	C	331	ARG
1	C	353	SER
1	C	354	ILE
1	C	357	SER
1	C	358	SER
1	C	366	LYS
1	C	371	LEU
1	C	380	SER
1	C	413	ARG
1	C	414	ARG
1	C	415	ILE
1	C	423	ASP
1	C	424	LEU
1	C	426	GLU
1	C	436	ASP
1	C	461	THR
1	C	470	ILE
1	D	140	LEU
1	D	142	LEU
1	D	143	GLU
1	D	146	LEU
1	D	148	GLN
1	D	149	ASP
1	D	150	LEU
1	D	153	SER
1	D	154	ASP
1	D	156	ILE
1	D	161	LEU
1	D	166	GLU
1	D	183	ASN
1	D	199	ASN
1	D	203	ILE
1	D	228	SER
1	D	302	LEU
1	D	309	GLU

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Mol	Chain	Res	Type
1	D	342	GLU
1	D	350	VAL
1	D	354	ILE
1	D	355	PHE
1	D	374	ASP
1	D	378	GLN
1	D	388	LEU
1	D	389	ASP
1	D	400	LEU
1	D	402	LEU
1	D	404	LEU
1	D	405	THR
1	D	425	ILE
1	D	463	VAL
1	D	471	THR
1	D	483	TRP
1	D	485	ASP
1	D	490	HIS
1	D	491	HIS
1	E	16	ASP
1	E	17	LEU
1	E	22	LEU
1	E	23	LEU
1	E	25	SER
1	E	26	LEU
1	E	43	CYS
1	E	80	LEU
1	E	83	LEU
1	E	87	THR
1	E	88	VAL
1	E	94	THR
1	E	96	PHE
1	E	99	ILE
1	E	103	CYS
1	E	107	GLU
1	E	112	ILE
1	E	120	LEU
1	E	121	PHE
1	E	125	ILE
1	E	128	LEU
1	E	171	ARG
1	E	174	HIS

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Mol	Chain	Res	Type
1	E	184	LEU
1	E	185	LEU
1	E	187	LEU
1	E	193	LEU
1	E	197	LEU
1	E	200	SER
1	E	209	SER
1	E	213	THR
1	E	220	ILE
1	E	224	ASP
1	E	228	SER
1	E	253	GLU
1	E	259	ASP
1	E	262	VAL
1	E	264	VAL
1	E	273	ASN
1	E	274	ASP
1	E	299	ILE
1	E	302	LEU
1	E	334	LYS
1	E	340	ARG
1	E	341	SER
1	E	355	PHE
1	E	356	SER
1	E	358	SER
1	E	363	GLN
1	E	366	LYS
1	E	371	LEU
1	E	374	ASP
1	E	376	THR
1	E	377	ILE
1	E	378	GLN
1	E	379	ILE
1	E	385	GLU
1	E	389	ASP
1	E	397	GLU
1	E	405	THR
1	E	415	ILE
1	E	417	TYR
1	E	419	ARG
1	E	460	LYS
1	E	466	THR

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Mol	Chain	Res	Type
1	E	485	ASP
1	F	10	LEU
1	F	14	THR
1	F	16	ASP
1	F	17	LEU
1	F	23	LEU
1	F	25	SER
1	F	26	LEU
1	F	29	LEU
1	F	54	PHE
1	F	57	PHE
1	F	59	GLU
1	F	60	LYS
1	F	62	LEU
1	F	63	ASP
1	F	64	ARG
1	F	69	ASP
1	F	70	ARG
1	F	83	LEU
1	F	87	THR
1	F	103	CYS
1	F	106	VAL
1	F	112	ILE
1	F	114	LEU
1	F	115	SER
1	F	116	THR
1	F	121	PHE
1	F	125	ILE
1	F	128	LEU
1	F	130	GLN
1	F	133	LEU
1	F	137	THR
1	F	143	GLU
1	F	146	LEU
1	F	154	ASP
1	F	161	LEU
1	F	178	LYS
1	F	183	ASN
1	F	185	LEU
1	F	200	SER
1	F	201	LYS
1	F	203	ILE

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Mol	Chain	Res	Type
1	F	213	THR
1	F	214	VAL
1	F	226	SER
1	F	231	ASP
1	F	257	VAL
1	F	278	THR
1	F	282	THR
1	F	332	THR
1	F	355	PHE
1	F	356	SER
1	F	358	SER
1	F	374	ASP
1	F	388	LEU
1	F	389	ASP
1	F	407	VAL
1	F	410	ASP
1	F	415	ILE
1	F	418	GLU
1	F	420	LEU
1	F	433	VAL
1	F	436	ASP
1	F	467	TRP
1	F	470	ILE
1	F	471	THR
1	F	482	THR
1	F	485	ASP
1	F	486	LEU
1	F	487	GLU
1	G	5	VAL
1	G	13	SER
1	G	21	MET
1	G	23	LEU
1	G	34	LEU
1	G	35	LEU
1	G	52	ASP
1	G	60	LYS
1	G	90	ILE
1	G	94	THR
1	G	99	ILE
1	G	102	LEU
1	G	106	VAL
1	G	112	ILE

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Mol	Chain	Res	Type
1	G	116	THR
1	G	117	SER
1	G	119	SER
1	G	122	GLU
1	G	125	ILE
1	G	128	LEU
1	G	130	GLN
1	G	142	LEU
1	G	144	LYS
1	G	150	LEU
1	G	154	ASP
1	G	171	ARG
1	G	200	SER
1	G	214	VAL
1	G	216	LEU
1	G	220	ILE
1	G	226	SER
1	G	228	SER
1	G	262	VAL
1	G	263	LYS
1	G	271	ILE
1	G	280	THR
1	G	290	SER
1	G	299	ILE
1	G	308	THR
1	G	309	GLU
1	G	330	ILE
1	G	355	PHE
1	G	356	SER
1	G	357	SER
1	G	358	SER
1	G	378	GLN
1	G	388	LEU
1	G	401	ASP
1	G	402	LEU
1	G	403	SER
1	G	405	THR
1	G	410	ASP
1	G	415	ILE
1	G	419	ARG
1	G	420	LEU
1	G	421	MET

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Mol	Chain	Res	Type
1	G	422	LEU
1	G	423	ASP
1	G	430	THR
1	G	463	VAL
1	G	466	THR
1	G	467	TRP
1	G	470	ILE
1	G	471	THR
1	G	473	ILE
1	G	476	VAL
1	G	486	LEU
1	H	13	SER
1	H	17	LEU
1	H	18	SER
1	H	25	SER
1	H	32	ASP
1	H	42	VAL
1	H	45	SER
1	H	46	ARG
1	H	50	ASP
1	H	91	THR
1	H	99	ILE
1	H	103	CYS
1	H	112	ILE
1	H	128	LEU
1	H	137	THR
1	H	142	LEU
1	H	143	GLU
1	H	148	GLN
1	H	156	ILE
1	H	168	GLN
1	H	171	ARG
1	H	174	HIS
1	H	183	ASN
1	H	214	VAL
1	H	220	ILE
1	H	224	ASP
1	H	225	SER
1	H	255	ASN
1	H	273	ASN
1	H	275	THR
1	H	276	VAL

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Mol	Chain	Res	Type
1	H	290	SER
1	H	341	SER
1	H	343	ILE
1	H	344	VAL
1	H	370	VAL
1	H	374	ASP
1	H	377	ILE
1	H	383	VAL
1	H	388	LEU
1	H	400	LEU
1	H	402	LEU
1	H	407	VAL
1	H	433	VAL
1	H	478	ARG
1	H	482	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	236	HIS
1	B	81	ASN
1	B	174	HIS
1	B	183	ASN
1	B	251	HIS
1	B	304	GLN
1	C	148	GLN
1	C	155	HIS
1	C	174	HIS
1	C	236	HIS
1	C	346	GLN
1	C	455	ASN
1	D	148	GLN
1	D	251	HIS
1	D	284	GLN
1	D	317	HIS
1	D	394	HIS
1	D	488	HIS
1	D	490	HIS
1	E	157	ASN
1	E	182	GLN
1	E	234	GLN

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Mol	Chain	Res	Type
1	E	304	GLN
1	E	346	GLN
1	E	394	HIS
1	E	441	GLN
1	F	72	ASN
1	F	168	GLN
1	F	234	GLN
1	F	239	GLN
1	F	273	ASN
1	F	317	HIS
1	F	346	GLN
1	G	130	GLN
1	G	148	GLN
1	G	205	HIS
1	G	207	GLN
1	G	352	HIS
1	G	365	ASN
1	G	378	GLN
1	G	394	HIS
1	H	191	ASN
1	H	234	GLN
1	H	365	ASN
1	H	441	GLN
1	H	455	ASN

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 ⓘ

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	451/493 (91%)	-1.31	0 100 100	34, 51, 95, 109	0
1	B	461/493 (93%)	-1.33	0 100 100	31, 48, 88, 114	0
1	C	345/493 (69%)	-1.33	0 100 100	37, 58, 73, 85	0
1	D	361/493 (73%)	-1.35	0 100 100	40, 58, 72, 83	0
1	E	446/493 (90%)	-1.27	0 100 100	36, 61, 83, 94	0
1	F	480/493 (97%)	-1.33	0 100 100	33, 59, 82, 98	0
1	G	465/493 (94%)	-1.35	0 100 100	32, 48, 85, 105	0
1	H	474/493 (96%)	-1.41	0 100 100	30, 47, 65, 79	0
All	All	3483/3944 (88%)	-1.34	0 100 100	30, 54, 83, 114	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.