



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:34 AM UTC

PDB ID : 8ZQA / pdb_00008zqa
Title : Crystal structure of 1,4-alpha-glucan branching protein from Rhodothermus profundus
Authors : Li, Q.; Zong, Z.Y.; Liu, W.D.
Deposited on : 2024-06-01
Resolution : 2.91 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

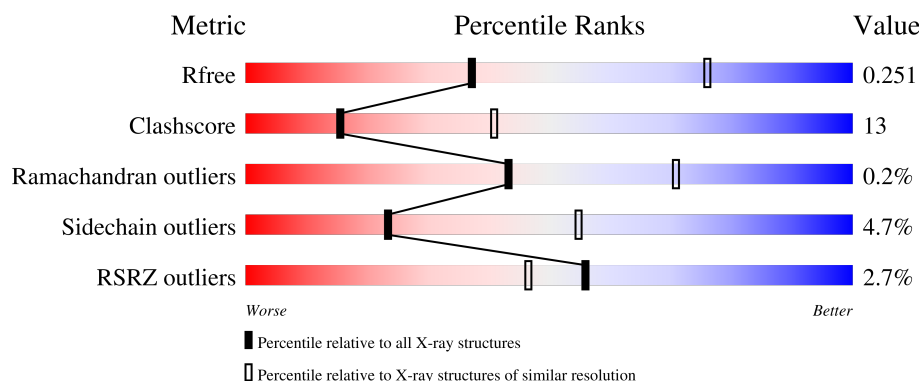
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	620	
1	B	620	
1	C	620	
1	D	620	
1	E	620	

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Mol	Chain	Length	Quality of chain
1	F	620	
1	G	620	
1	H	620	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 39395 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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	0	0	0
			4886	3190	817	865	14			
1	B	603	Total	C	N	O	S	0	0	0
			4925	3212	832	867	14			
1	C	606	Total	C	N	O	S	0	0	0
			4925	3209	826	875	15			
1	D	599	Total	C	N	O	S	0	0	0
			4888	3186	822	866	14			
1	E	604	Total	C	N	O	S	0	0	0
			4917	3202	830	871	14			
1	F	593	Total	C	N	O	S	0	0	0
			4859	3166	818	861	14			
1	G	606	Total	C	N	O	S	0	0	0
			4923	3213	826	869	15			
1	H	603	Total	C	N	O	S	0	0	0
			4800	3138	791	857	14			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total	O	0	0
			45	45		
2	B	34	Total	O	0	0
			34	34		
2	C	31	Total	O	0	0
			31	31		
2	D	27	Total	O	0	0
			27	27		
2	E	26	Total	O	0	0
			26	26		
2	F	51	Total	O	0	0
			51	51		

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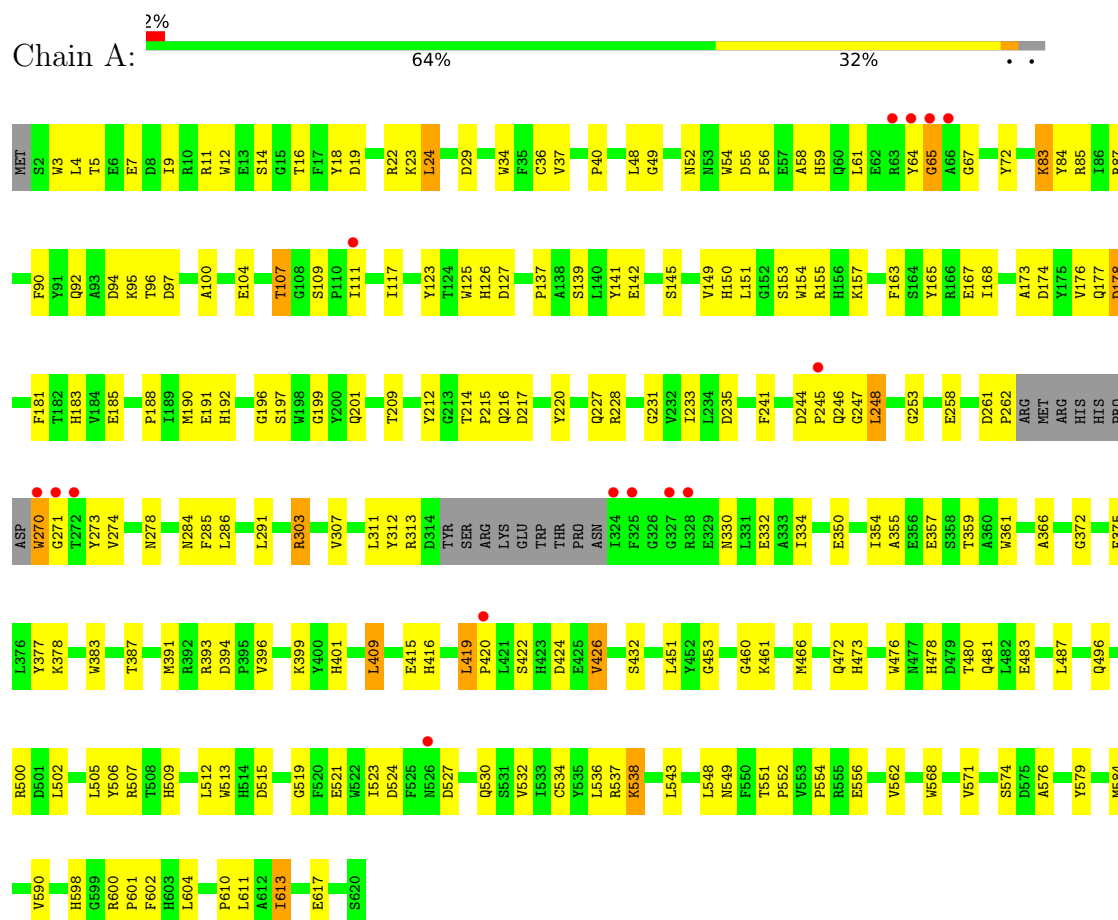
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	34	Total 34	O 34	0	0
2	H	24	Total 24	O 24	0	0

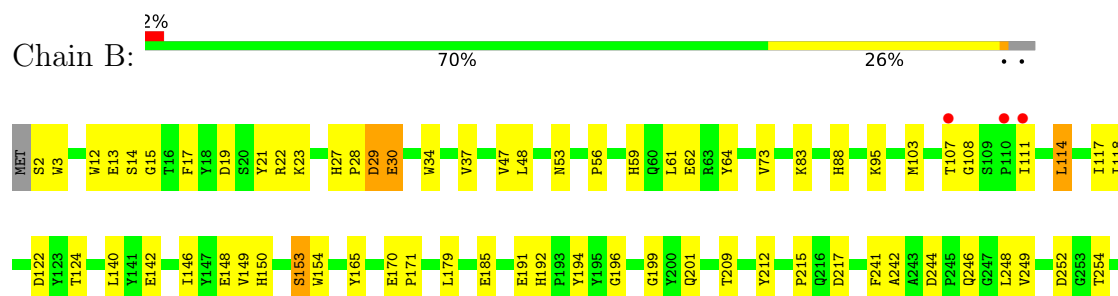
3 Residue-property plots

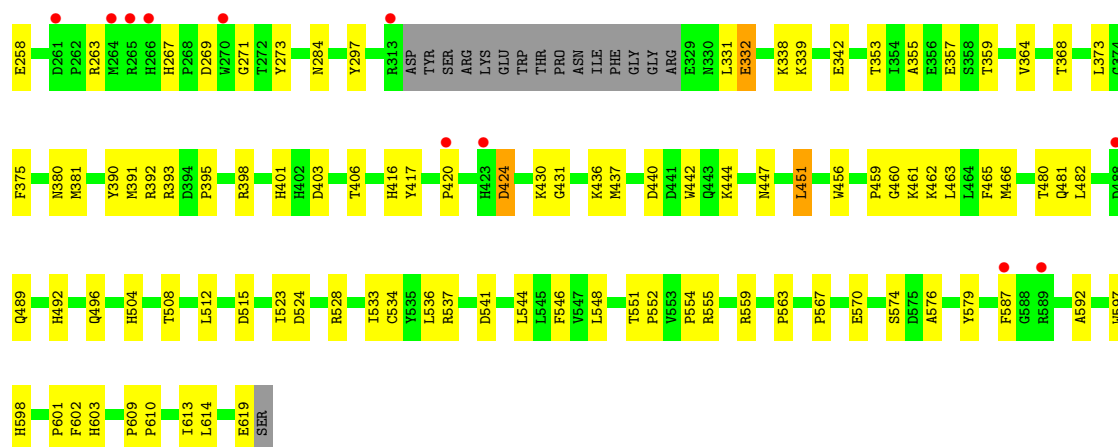
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 1,4-alpha-glucan branching enzyme GlgB

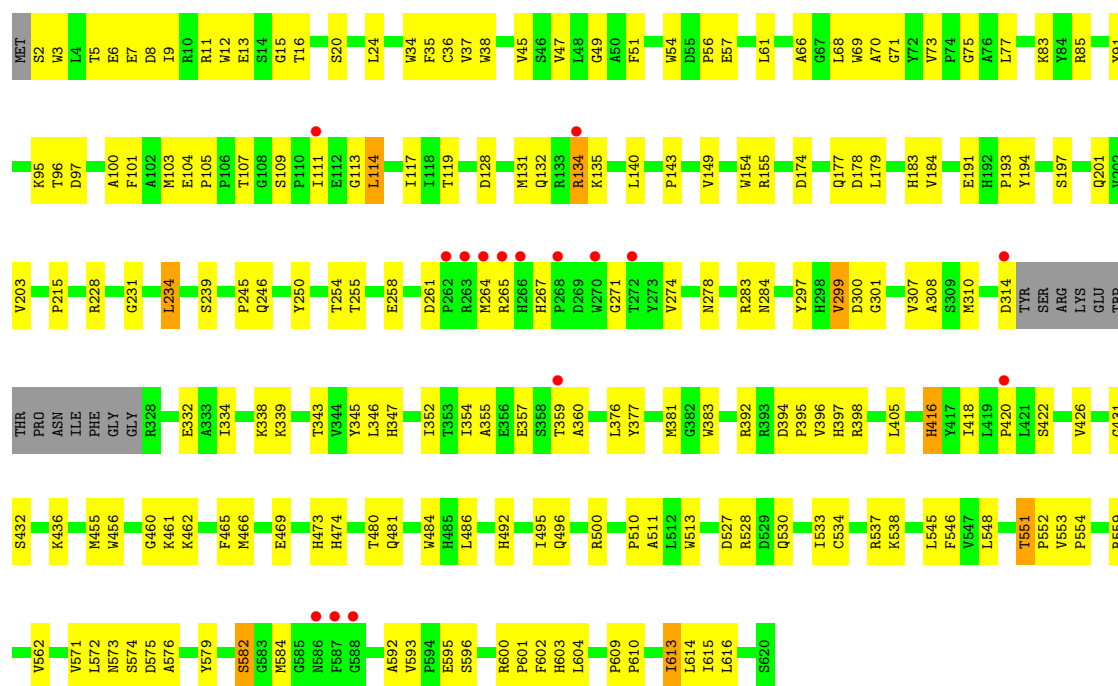


- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

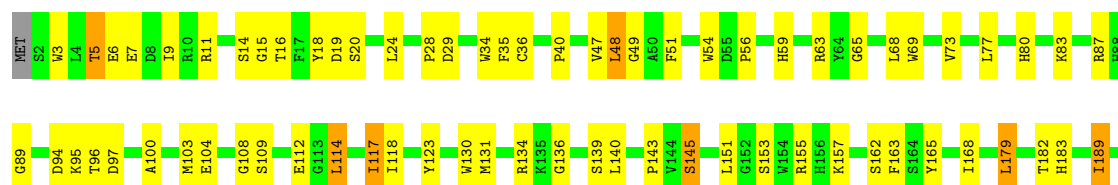


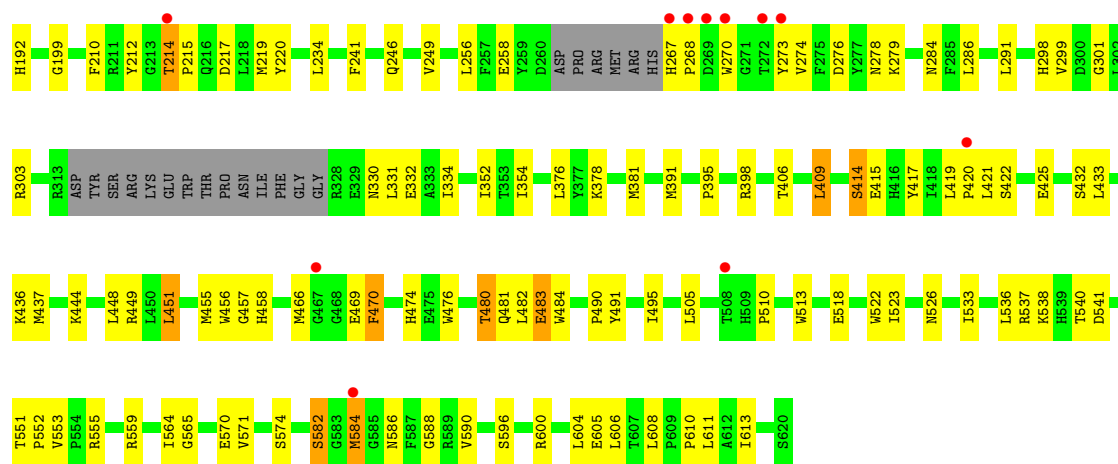


- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

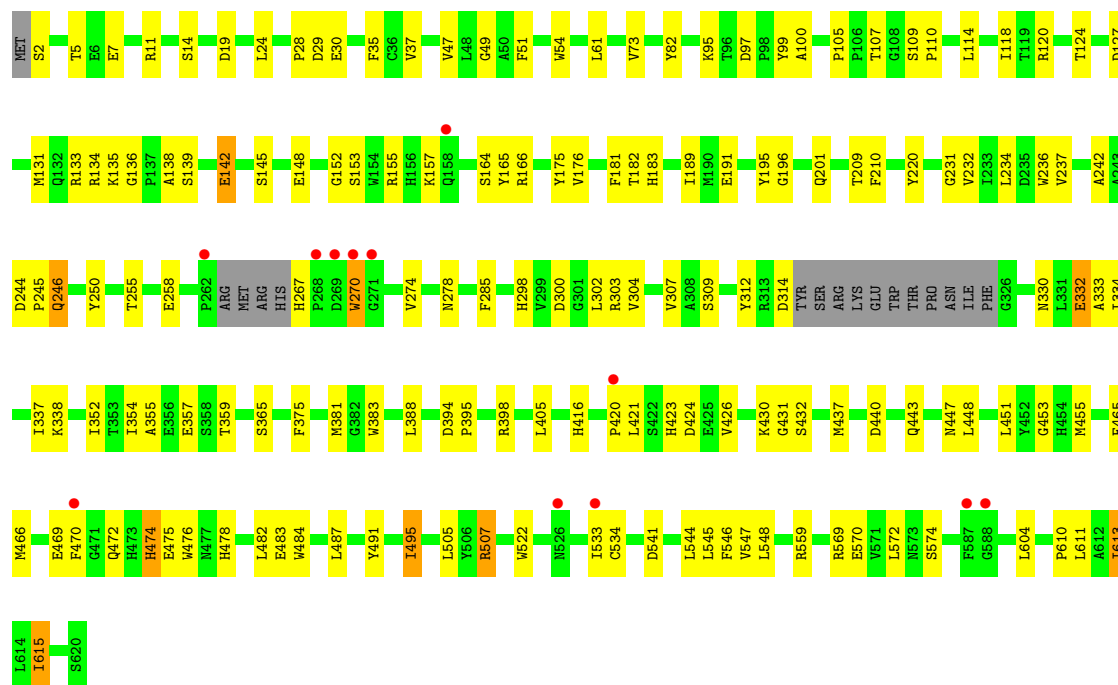


- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

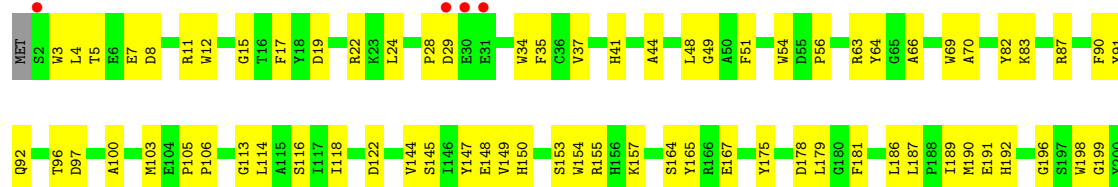


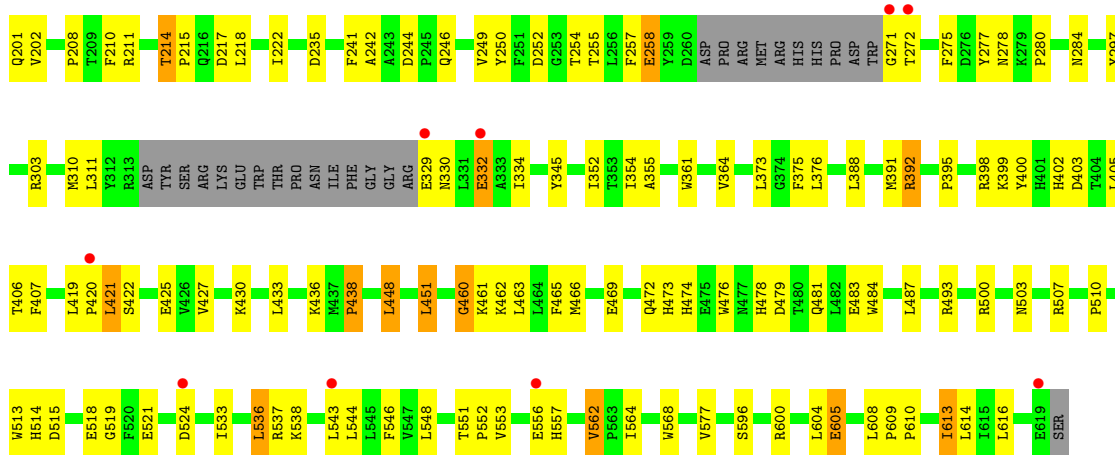


• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

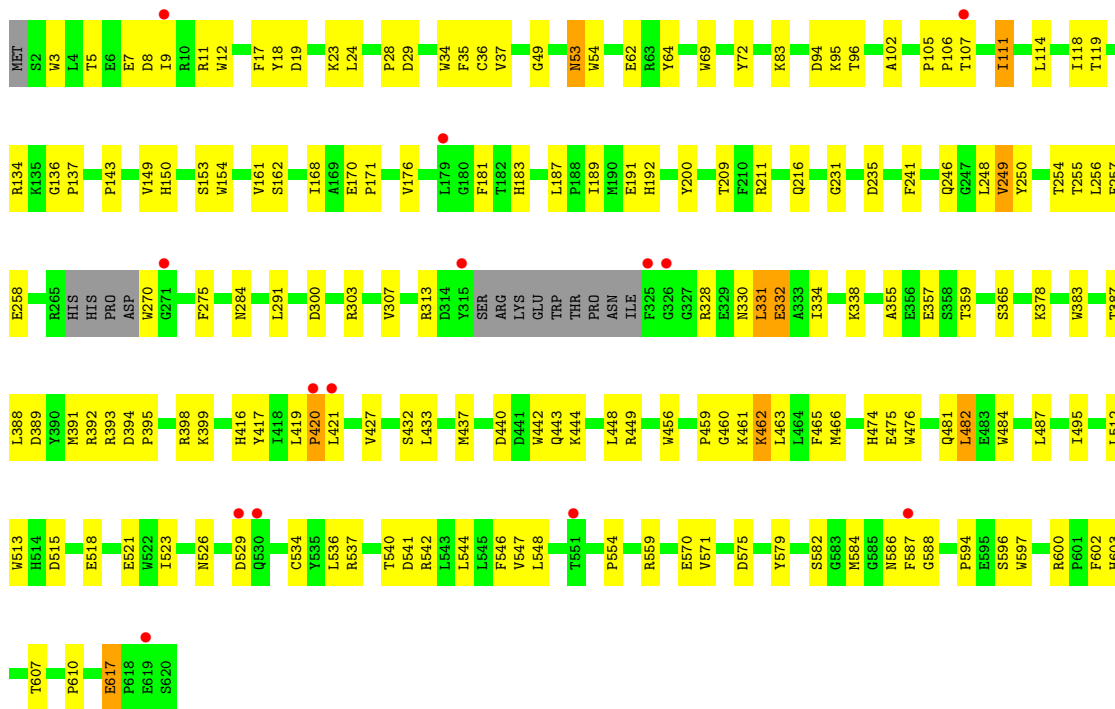


• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

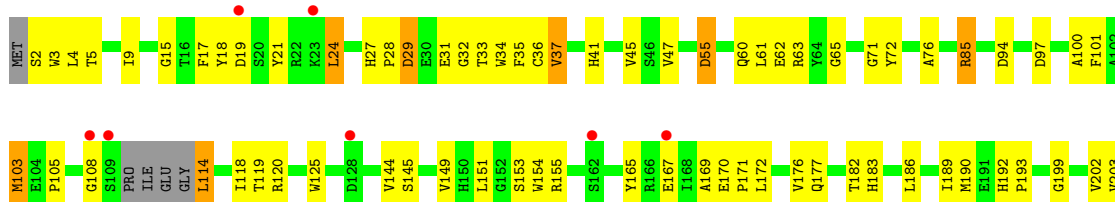


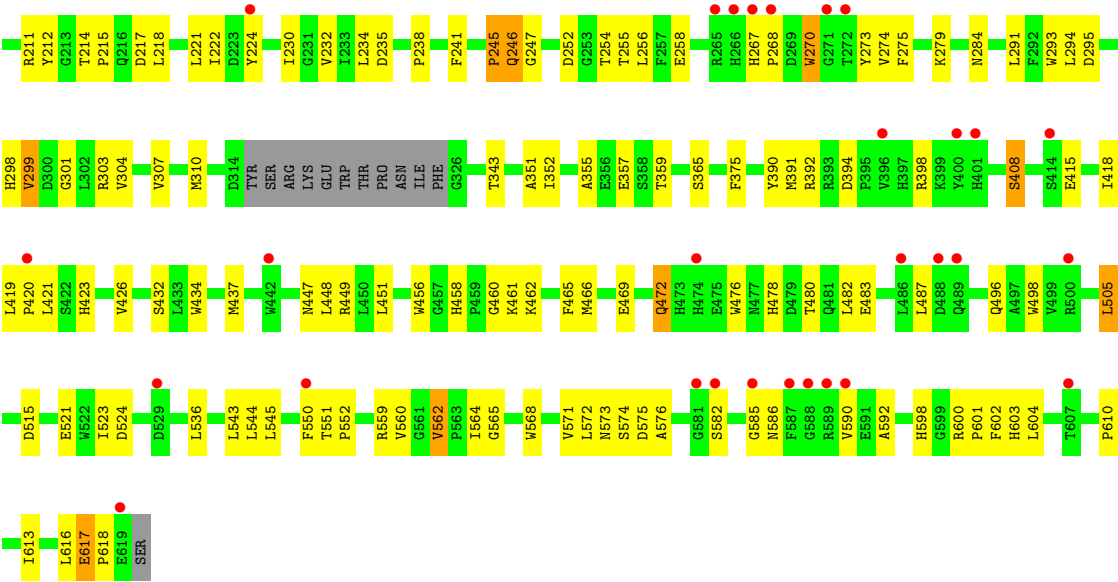


• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	100.30Å 112.27Å 166.26Å 73.59° 73.77° 65.25°	Depositor
Resolution (Å)	100.10 – 2.91 100.10 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.9 (100.10-2.91) 98.9 (100.10-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.197 , 0.256 (Not available) , 0.251	Depositor DCC
R_{free} test set	6764 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.012 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	39395	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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	0.43	0/5080	0.75	7/6952 (0.1%)
1	B	0.35	0/5123	0.66	5/7011 (0.1%)
1	C	0.39	0/5121	0.69	3/7009 (0.0%)
1	D	0.41	0/5082	0.70	4/6952 (0.1%)
1	E	0.35	0/5112	0.65	3/6993 (0.0%)
1	F	0.38	0/5049	0.65	4/6902 (0.1%)
1	G	0.40	0/5118	0.72	3/7000 (0.0%)
1	H	0.50	0/4993	0.83	9/6851 (0.1%)
All	All	0.40	0/40678	0.71	38/55670 (0.1%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	55	ASP	CB-CA-C	7.04	117.78	109.47
1	E	416	HIS	N-CA-C	-6.75	99.67	109.59
1	A	245	PRO	N-CA-C	-6.67	104.27	113.53
1	A	416	HIS	N-CA-C	-6.57	99.20	109.25
1	H	19	ASP	N-CA-C	-6.33	104.86	112.59
1	G	588	GLY	N-CA-C	-6.06	107.04	114.92
1	F	460	GLY	CA-C-O	-6.01	118.31	122.22
1	G	416	HIS	N-CA-C	-5.96	99.43	108.67
1	H	18	TYR	CB-CA-C	5.89	119.93	110.09
1	H	108	GLY	N-CA-C	-5.79	107.33	115.32
1	D	108	GLY	N-CA-C	-5.78	107.05	114.85
1	D	5	THR	OG1-CB-CG2	5.77	120.83	109.30
1	B	15	GLY	N-CA-C	-5.72	106.57	115.67
1	D	273	TYR	CB-CA-C	5.69	120.33	110.72
1	H	273	TYR	N-CA-C	-5.64	105.35	114.09
1	H	421	LEU	N-CA-C	-5.55	99.47	108.52
1	A	273	TYR	CB-CA-C	5.53	120.07	110.72
1	F	438	PRO	N-CA-C	5.53	119.98	111.57
1	B	263	ARG	CA-C-N	-5.52	111.00	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	ARG	C-N-CA	-5.52	111.00	121.54
1	D	586	ASN	N-CA-C	-5.50	106.41	113.23
1	E	165	TYR	CB-CA-C	-5.48	101.70	110.79
1	A	285	PHE	N-CA-CB	-5.43	102.14	110.12
1	E	495	ILE	CA-CB-CG1	5.38	119.55	110.40
1	A	271	GLY	CA-C-O	-5.36	116.69	121.41
1	B	108	GLY	N-CA-C	-5.34	108.27	115.21
1	B	29	ASP	N-CA-C	-5.32	101.28	109.52
1	H	586	ASN	N-CA-C	-5.27	105.54	111.28
1	A	65	GLY	CA-C-N	-5.18	114.28	121.99
1	A	65	GLY	C-N-CA	-5.18	114.28	121.99
1	F	421	LEU	N-CA-C	-5.17	100.48	108.90
1	G	460	GLY	CA-C-O	-5.17	118.67	122.23
1	C	416	HIS	N-CA-C	-5.15	101.36	109.25
1	C	265	ARG	CA-C-N	-5.13	115.38	122.30
1	C	265	ARG	C-N-CA	-5.13	115.38	122.30
1	H	55	ASP	CA-CB-CG	5.11	117.71	112.60
1	F	430	LYS	N-CA-C	-5.10	105.72	111.28
1	H	245	PRO	N-CA-C	5.02	120.51	113.53

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	4886	0	4484	128	0
1	B	4925	0	4535	118	0
1	C	4925	0	4517	124	0
1	D	4888	0	4499	120	0
1	E	4917	0	4523	117	0
1	F	4859	0	4500	131	0
1	G	4923	0	4527	118	0
1	H	4800	0	4320	163	0
2	A	45	0	0	3	0
2	B	34	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	0	0	0
2	D	27	0	0	0	0
2	E	26	0	0	1	0
2	F	51	0	0	1	0
2	G	34	0	0	1	0
2	H	24	0	0	1	0
All	All	39395	0	35905	1007	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 13.

All (1007) 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:D:5:THR:HG22	1:D:7:GLU:H	1.16	1.05
1:F:15:GLY:HA2	1:F:284:ASN:HD21	1.33	0.94
1:H:145:SER:H	1:H:182:THR:HG22	1.38	0.87
1:C:426:VAL:HG13	1:C:432:SER:HA	1.57	0.87
1:H:120:ARG:HB2	1:H:120:ARG:HH11	1.38	0.87
1:E:29:ASP:OD1	1:E:30:GLU:N	2.07	0.87
1:E:110:PRO:HG3	1:E:210:PHE:HZ	1.41	0.86
1:B:124:THR:HG21	1:E:541:ASP:HB2	1.57	0.84
1:D:5:THR:HG22	1:D:7:GLU:N	1.93	0.84
1:D:391:MET:HE2	1:D:451:LEU:HB2	1.61	0.83
1:F:258:GLU:N	1:F:258:GLU:OE1	2.11	0.82
1:H:574:SER:HB3	1:H:613:ILE:H	1.43	0.82
1:E:357:GLU:OE2	1:E:359:THR:HB	1.80	0.81
1:D:83:LYS:HD2	1:D:94:ASP:HB3	1.62	0.81
1:H:456:TRP:HA	1:H:462:LYS:HE3	1.61	0.81
1:G:523:ILE:HD11	1:G:536:LEU:HG	1.64	0.80
1:H:562:VAL:HG23	1:H:602:PHE:HB2	1.65	0.79
1:D:145:SER:H	1:D:182:THR:HB	1.48	0.78
1:H:154:TRP:HD1	1:H:466:MET:HE2	1.48	0.78
1:E:47:VAL:HG23	1:E:61:LEU:HD21	1.64	0.78
1:H:144:VAL:HG23	1:H:461:LYS:HB3	1.63	0.78
1:F:551:THR:HG22	1:F:553:VAL:H	1.48	0.78
1:B:554:PRO:HG3	1:B:610:PRO:HG3	1.65	0.77
1:C:456:TRP:HA	1:C:462:LYS:HE3	1.66	0.77
1:B:541:ASP:HB2	1:E:124:THR:HG21	1.65	0.77
1:B:357:GLU:OE2	1:B:359:THR:HB	1.83	0.77
1:H:144:VAL:HA	1:H:182:THR:HG21	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ARG:HA	1:D:481:GLN:HG3	1.66	0.76
1:D:182:THR:HG22	1:D:183:HIS:ND1	1.99	0.76
1:B:437:MET:HE3	1:B:447:ASN:HB3	1.68	0.75
1:A:523:ILE:HD11	1:A:536:LEU:HD22	1.67	0.75
1:E:470:PHE:HZ	1:E:484:TRP:CZ3	2.06	0.74
1:F:19:ASP:OD2	1:F:22:ARG:NH2	2.20	0.74
1:G:17:PHE:HE1	1:G:19:ASP:HB2	1.52	0.74
1:E:466:MET:HB3	1:E:482:LEU:HD11	1.70	0.73
1:F:155:ARG:HA	1:F:481:GLN:HG3	1.71	0.73
1:H:144:VAL:CG2	1:H:461:LYS:HB3	2.17	0.73
1:E:28:PRO:HG3	1:E:118:ILE:HG22	1.71	0.73
1:G:540:THR:HG22	1:G:541:ASP:H	1.54	0.73
1:H:466:MET:HB2	1:H:482:LEU:HD11	1.70	0.73
1:F:149:VAL:HA	1:F:466:MET:HE3	1.70	0.72
1:D:352:ILE:HG23	1:D:376:LEU:HD23	1.72	0.72
1:G:466:MET:HE3	1:G:482:LEU:HD21	1.70	0.72
1:H:9:ILE:HG21	1:H:65:GLY:HA3	1.70	0.71
1:H:559:ARG:HG2	1:H:603:HIS:CD2	2.25	0.71
1:B:466:MET:HB2	1:B:482:LEU:HD11	1.71	0.71
1:E:5:THR:HG22	1:E:7:GLU:H	1.56	0.71
1:H:521:GLU:HG2	1:H:600:ARG:HH22	1.56	0.71
1:A:126:HIS:HB2	1:A:227:GLN:OE1	1.91	0.71
1:E:533:ILE:HG23	1:E:548:LEU:HB2	1.73	0.70
1:F:103:MET:HE2	1:F:191:GLU:HG2	1.74	0.70
1:B:19:ASP:OD2	1:B:22:ARG:NH2	2.21	0.70
1:B:338:LYS:HG2	1:B:368:THR:HG22	1.74	0.69
1:C:131:MET:HA	1:C:134:ARG:HG3	1.73	0.69
1:D:470:PHE:HZ	1:D:484:TRP:CZ3	2.09	0.69
1:B:570:GLU:OE2	1:B:614:LEU:HD23	1.92	0.69
1:F:303:ARG:HG2	1:F:354:ILE:HB	1.72	0.69
1:A:357:GLU:OE2	1:A:359:THR:HB	1.92	0.69
1:D:131:MET:HA	1:D:134:ARG:HG3	1.74	0.69
1:H:437:MET:HG3	1:H:447:ASN:HB3	1.75	0.69
1:D:87:ARG:NH1	1:D:89:GLY:O	2.25	0.69
1:B:574:SER:HB3	1:B:613:ILE:HG22	1.75	0.68
1:E:97:ASP:HB3	1:E:100:ALA:HB2	1.74	0.68
1:G:357:GLU:OE2	1:G:359:THR:HB	1.93	0.68
1:F:391:MET:HE2	1:F:451:LEU:HB2	1.74	0.68
1:E:189:ILE:HD11	1:E:234:LEU:HD13	1.76	0.68
1:G:62:GLU:HG3	1:G:64:TYR:HE1	1.59	0.68
1:F:5:THR:HG22	1:F:8:ASP:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:THR:HG22	1:G:7:GLU:H	1.59	0.67
1:G:442:TRP:HE3	1:G:443:GLN:HG3	1.59	0.67
1:H:145:SER:H	1:H:182:THR:CG2	2.06	0.67
1:D:395:PRO:HA	1:D:398:ARG:HD2	1.76	0.67
1:E:131:MET:HA	1:E:134:ARG:HG3	1.77	0.67
1:H:357:GLU:OE2	1:H:359:THR:HB	1.95	0.67
1:C:234:LEU:HD22	1:C:299:VAL:HG11	1.76	0.67
1:H:149:VAL:HA	1:H:466:MET:HE3	1.77	0.67
1:H:33:THR:HG21	1:H:118:ILE:HG21	1.77	0.67
1:H:193:PRO:HD3	1:H:203:VAL:HG13	1.75	0.67
1:A:307:VAL:HG21	1:A:355:ALA:HB1	1.77	0.67
1:B:548:LEU:HG	1:B:613:ILE:HG13	1.76	0.67
1:E:383:TRP:CH2	1:E:455:MET:HG3	2.29	0.67
1:G:378:LYS:HD3	1:G:417:TYR:HE1	1.60	0.67
1:H:255:THR:HA	1:H:258:GLU:OE1	1.94	0.66
1:B:165:TYR:HB2	1:B:217:ASP:HB3	1.75	0.66
1:H:144:VAL:HG22	1:H:461:LYS:HD2	1.77	0.66
1:C:554:PRO:HD3	1:C:610:PRO:HG3	1.76	0.66
1:G:448:LEU:HD23	1:G:495:ILE:HD13	1.76	0.66
1:E:183:HIS:CD2	1:E:231:GLY:HA3	2.30	0.66
1:F:198:TRP:HH2	1:F:427:VAL:HG21	1.60	0.66
1:G:153:SER:HB2	1:G:466:MET:HE1	1.76	0.66
1:F:17:PHE:N	1:F:284:ASN:OD1	2.28	0.66
1:B:149:VAL:HA	1:B:466:MET:HE3	1.77	0.66
1:D:189:ILE:HD11	1:D:234:LEU:HD13	1.78	0.66
1:E:139:SER:HA	1:E:142:GLU:HG3	1.77	0.66
1:F:165:TYR:HB2	1:F:217:ASP:HB3	1.77	0.66
1:E:145:SER:H	1:E:182:THR:HB	1.60	0.65
1:F:63:ARG:NH1	1:F:64:TYR:O	2.29	0.65
1:F:518:GLU:HG3	1:F:519:GLY:H	1.60	0.65
1:H:437:MET:HG3	1:H:447:ASN:CB	2.26	0.65
1:E:11:ARG:NH2	1:E:19:ASP:OD1	2.29	0.65
1:F:241:PHE:HB3	1:F:275:PHE:CZ	2.32	0.65
1:H:469:GLU:OE1	1:H:469:GLU:N	2.22	0.65
1:B:142:GLU:OE2	1:E:133:ARG:HD3	1.96	0.65
1:D:24:LEU:HA	1:D:36:CYS:HB3	1.78	0.65
1:E:182:THR:HG22	1:E:183:HIS:ND1	2.11	0.65
1:G:313:ARG:HG3	1:G:328:ARG:O	1.97	0.65
1:C:352:ILE:HG23	1:C:376:LEU:HD23	1.78	0.65
1:C:562:VAL:HG23	1:C:602:PHE:HB2	1.79	0.65
1:D:28:PRO:HG3	1:D:118:ILE:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:405:LEU:HD21	1:F:533:ILE:HG13	1.79	0.64
1:C:545:LEU:HD23	1:C:616:LEU:HD13	1.79	0.64
1:F:474:HIS:ND1	1:F:483:GLU:OE2	2.29	0.64
1:G:554:PRO:HG3	1:G:610:PRO:HG3	1.80	0.64
1:F:178:ASP:CG	1:F:500:ARG:HH21	2.06	0.64
1:H:9:ILE:HD13	1:H:65:GLY:H	1.63	0.64
1:H:568:TRP:CD1	1:H:604:LEU:HD21	2.33	0.64
1:H:408:SER:OG	1:H:458:HIS:NE2	2.30	0.63
1:E:303:ARG:HG2	1:E:354:ILE:HB	1.81	0.63
1:G:587:PHE:HA	2:G:718:HOH:O	1.99	0.63
1:H:165:TYR:HB2	1:H:217:ASP:HB3	1.80	0.63
1:A:19:ASP:HB3	1:A:22:ARG:HD3	1.79	0.63
1:F:254:THR:HG22	1:F:255:THR:H	1.64	0.63
1:H:154:TRP:CD1	1:H:466:MET:HE2	2.34	0.63
1:E:574:SER:HB3	1:E:613:ILE:H	1.63	0.63
1:H:505:LEU:HD11	1:H:544:LEU:HD21	1.81	0.63
1:H:153:SER:OG	1:H:478:HIS:HA	1.98	0.63
1:A:554:PRO:HB3	1:A:584:MET:HE1	1.79	0.62
1:D:6:GLU:CD	1:D:6:GLU:H	2.05	0.62
1:F:395:PRO:HA	1:F:398:ARG:HD2	1.79	0.62
1:A:155:ARG:HA	1:A:481:GLN:HG3	1.81	0.62
1:G:24:LEU:HA	1:G:36:CYS:HB3	1.81	0.62
1:H:120:ARG:HB2	1:H:120:ARG:NH1	2.13	0.62
1:H:434:TRP:HA	1:H:448:LEU:HD11	1.81	0.62
1:A:519:GLY:O	1:A:537:ARG:HA	1.99	0.62
1:A:5:THR:O	1:A:9:ILE:HD12	1.98	0.62
1:C:177:GLN:OE1	1:C:228:ARG:NH2	2.29	0.62
1:G:334:ILE:HG22	1:G:338:LYS:HD2	1.81	0.62
1:C:183:HIS:CD2	1:C:231:GLY:HA3	2.35	0.62
1:H:154:TRP:CH2	1:H:172:LEU:HA	2.34	0.62
1:C:250:TYR:HA	1:C:254:THR:O	1.99	0.62
1:C:239:SER:HB3	1:C:310:MET:HE2	1.82	0.61
1:C:574:SER:HB3	1:C:613:ILE:CG2	2.30	0.61
1:G:559:ARG:HB3	1:G:603:HIS:CD2	2.35	0.61
1:C:575:ASP:OD2	1:C:609:PRO:HB3	2.01	0.61
1:B:504:HIS:O	1:B:508:THR:HG23	2.00	0.61
1:D:522:TRP:HZ3	1:D:533:ILE:HG23	1.65	0.61
1:D:582:SER:HB2	1:D:584:MET:HE3	1.81	0.61
1:C:6:GLU:CD	1:C:6:GLU:H	2.08	0.61
1:D:303:ARG:HG2	1:D:354:ILE:HB	1.82	0.61
1:C:154:TRP:HD1	1:C:466:MET:HE2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:291:LEU:HD21	1:H:343:THR:HG22	1.83	0.61
1:G:153:SER:O	1:G:481:GLN:HA	2.01	0.61
1:G:313:ARG:HG2	1:G:330:ASN:HB2	1.83	0.60
1:A:3:TRP:H	1:A:64:TYR:HE2	1.48	0.60
1:C:551:THR:CG2	1:C:553:VAL:HG22	2.32	0.60
1:G:440:ASP:O	1:G:444:LYS:HG3	2.01	0.60
1:C:95:LYS:NZ	1:C:245:PRO:O	2.34	0.60
1:F:257:PHE:N	1:F:258:GLU:OE1	2.35	0.60
1:H:304:VAL:HG12	1:H:307:VAL:HG22	1.83	0.60
1:H:97:ASP:HB3	1:H:100:ALA:HB2	1.83	0.60
1:D:95:LYS:NZ	1:D:249:VAL:O	2.35	0.60
1:A:378:LYS:HD3	1:A:415:GLU:HG3	1.84	0.59
1:A:48:LEU:HD11	1:A:56:PRO:HA	1.85	0.59
1:A:303:ARG:HG3	1:A:354:ILE:HB	1.84	0.59
1:F:15:GLY:CA	1:F:284:ASN:HD21	2.13	0.59
1:E:470:PHE:CZ	1:E:484:TRP:CZ3	2.90	0.59
1:F:48:LEU:HD21	1:F:56:PRO:HA	1.83	0.59
1:H:190:MET:HE1	1:H:235:ASP:O	2.02	0.59
1:C:527:ASP:OD1	1:C:530:GLN:HB2	2.02	0.59
1:E:443:GLN:O	1:E:447:ASN:ND2	2.35	0.59
1:G:255:THR:HG22	1:G:258:GLU:HB2	1.85	0.59
1:F:148:GLU:HB3	1:F:465:PHE:HA	1.85	0.59
1:B:524:ASP:HB2	1:B:598:HIS:CD2	2.38	0.58
1:H:15:GLY:HA2	1:H:284:ASN:OD1	2.03	0.58
1:F:521:GLU:OE1	1:F:600:ARG:NH2	2.32	0.58
1:B:523:ILE:HD11	1:B:536:LEU:HD13	1.86	0.58
1:G:389:ASP:OD2	1:G:393:ARG:NH2	2.37	0.58
1:H:398:ARG:NH1	1:H:550:PHE:O	2.36	0.58
1:H:545:LEU:HD23	1:H:616:LEU:HD23	1.83	0.58
1:D:109:SER:HB3	1:D:112:GLU:HG3	1.85	0.58
1:A:96:THR:HG22	1:C:91:TYR:OH	2.03	0.58
1:B:609:PRO:HD2	1:B:614:LEU:HD11	1.85	0.58
1:C:346:LEU:HD23	1:C:347:HIS:CE1	2.38	0.58
1:D:131:MET:HG2	1:D:134:ARG:HD3	1.86	0.58
1:F:208:PRO:HB3	1:F:218:LEU:HD22	1.85	0.58
1:F:258:GLU:H	1:F:258:GLU:CD	2.10	0.58
1:G:383:TRP:O	1:G:387:THR:OG1	2.21	0.58
1:G:512:LEU:HD23	1:G:537:ARG:HG2	1.84	0.58
1:H:182:THR:HG23	1:H:183:HIS:ND1	2.19	0.58
1:D:153:SER:HB2	1:D:466:MET:HE1	1.86	0.58
1:F:192:HIS:O	1:F:211:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:ASP:OD1	1:G:72:TYR:HE1	1.87	0.58
1:G:388:LEU:O	1:G:392:ARG:HG3	2.04	0.58
1:A:521:GLU:OE2	1:A:600:ARG:NH1	2.36	0.58
1:D:48:LEU:HD21	1:D:56:PRO:HA	1.85	0.58
1:H:466:MET:HB2	1:H:482:LEU:CD1	2.33	0.58
1:G:192:HIS:CE1	1:G:211:ARG:HH22	2.22	0.58
1:A:24:LEU:HA	1:A:36:CYS:HB3	1.86	0.57
1:B:47:VAL:HG23	1:B:61:LEU:HD21	1.86	0.57
1:B:48:LEU:HB2	1:B:83:LYS:HG3	1.86	0.57
1:G:518:GLU:CD	1:G:518:GLU:H	2.11	0.57
1:A:177:GLN:HE22	1:A:228:ARG:HE	1.51	0.57
1:C:104:GLU:HG3	1:C:117:ILE:HD13	1.86	0.57
1:F:564:ILE:HG22	1:F:568:TRP:CZ2	2.39	0.57
1:A:177:GLN:NE2	1:A:228:ARG:HE	2.03	0.57
1:E:47:VAL:CG2	1:E:61:LEU:HD21	2.34	0.57
1:D:552:PRO:HG3	1:D:611:LEU:HD11	1.86	0.57
1:F:244:ASP:OD2	1:F:246:GLN:N	2.38	0.57
1:B:391:MET:HE2	1:B:451:LEU:HB2	1.85	0.57
1:C:551:THR:HG21	1:C:553:VAL:HG22	1.87	0.57
1:E:522:TRP:CH2	1:E:533:ILE:HD11	2.39	0.57
1:F:41:HIS:ND1	1:F:252:ASP:OD2	2.38	0.57
1:A:85:ARG:HD3	1:A:94:ASP:OD1	2.05	0.57
1:D:63:ARG:HD2	1:D:69:TRP:CZ2	2.40	0.57
1:E:110:PRO:HG3	1:E:210:PHE:CZ	2.32	0.57
1:F:48:LEU:HB2	1:F:83:LYS:HG2	1.86	0.57
1:G:440:ASP:OD2	1:G:443:GLN:NE2	2.38	0.57
1:G:442:TRP:HH2	1:G:610:PRO:HB2	1.70	0.57
1:H:241:PHE:HZ	1:H:258:GLU:HG3	1.70	0.57
1:B:244:ASP:HB3	1:B:246:GLN:HE22	1.70	0.56
1:C:486:LEU:HB3	1:C:492:HIS:ND1	2.20	0.56
1:D:551:THR:HG21	1:D:555:ARG:HH21	1.70	0.56
1:D:555:ARG:HB2	1:D:608:LEU:HB2	1.85	0.56
1:C:308:ALA:HB2	1:C:357:GLU:OE2	2.04	0.56
1:C:339:LYS:O	1:C:343:THR:HG23	2.05	0.56
1:G:3:TRP:HB2	1:G:34:TRP:CZ3	2.40	0.56
1:G:95:LYS:NZ	1:G:249:VAL:O	2.33	0.56
1:H:28:PRO:HG3	1:H:118:ILE:HG22	1.87	0.56
1:A:153:SER:HB2	1:A:466:MET:HE1	1.87	0.56
1:C:460:GLY:O	1:C:462:LYS:NZ	2.26	0.56
1:B:559:ARG:HB3	1:B:603:HIS:CD2	2.40	0.56
1:D:256:LEU:O	1:D:279:LYS:NZ	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:546:PHE:HD2	1:E:613:ILE:HD11	1.70	0.56
1:G:241:PHE:HZ	1:G:258:GLU:HG3	1.70	0.56
1:B:267:HIS:HE1	1:B:269:ASP:HB2	1.71	0.56
1:B:440:ASP:O	1:B:444:LYS:HG3	2.06	0.56
1:E:267:HIS:CE1	1:E:309:SER:HB2	2.41	0.56
1:F:518:GLU:HG3	1:F:519:GLY:N	2.20	0.56
1:G:437:MET:O	1:G:444:LYS:HE3	2.05	0.56
1:H:307:VAL:HG21	1:H:355:ALA:HB1	1.88	0.56
1:F:49:GLY:HA3	1:F:51:PHE:CE1	2.41	0.56
1:F:388:LEU:O	1:F:392:ARG:HG3	2.05	0.56
1:G:102:ALA:HB3	1:G:119:THR:HG21	1.88	0.56
1:A:52:ASN:HD22	1:A:59:HIS:HD2	1.54	0.56
1:B:597:TRP:HD1	1:B:598:HIS:ND1	2.04	0.56
1:B:154:TRP:HB2	1:B:466:MET:HE1	1.88	0.56
1:C:149:VAL:HA	1:C:466:MET:HE3	1.88	0.55
1:E:432:SER:OG	1:E:472:GLN:O	2.23	0.55
1:F:577:VAL:HG22	2:F:709:HOH:O	2.05	0.55
1:A:241:PHE:HZ	1:A:258:GLU:HG3	1.72	0.55
1:F:419:LEU:N	1:F:461:LYS:O	2.36	0.55
1:A:157:LYS:HG2	1:A:163:PHE:CE1	2.41	0.55
1:F:5:THR:HG22	1:F:8:ASP:N	2.21	0.55
1:H:192:HIS:CD2	1:H:199:GLY:HA2	2.41	0.55
1:B:576:ALA:HB3	1:B:579:TYR:CD2	2.42	0.55
1:G:216:GLN:CD	1:G:216:GLN:H	2.15	0.55
1:A:584:MET:HE2	1:A:610:PRO:HD3	1.87	0.55
1:E:333:ALA:O	1:E:337:ILE:HG13	2.06	0.55
1:H:214:THR:HG22	1:H:215:PRO:HD2	1.89	0.55
1:B:154:TRP:HD1	1:B:466:MET:HE2	1.70	0.55
1:C:155:ARG:HG2	1:C:484:TRP:NE1	2.22	0.55
1:E:153:SER:HB2	1:E:466:MET:HE1	1.89	0.55
1:G:594:PRO:HA	1:G:602:PHE:CD1	2.41	0.55
1:F:5:THR:HG23	1:F:7:GLU:H	1.71	0.55
1:C:51:PHE:CD1	1:C:73:VAL:HG11	2.42	0.55
1:F:147:TYR:OH	1:F:469:GLU:OE2	2.21	0.55
1:C:37:VAL:HG11	1:C:45:VAL:HG11	1.89	0.55
1:C:574:SER:HB3	1:C:613:ILE:HG22	1.89	0.55
1:E:232:VAL:N	1:E:300:ASP:OD2	2.30	0.55
1:D:470:PHE:CZ	1:D:484:TRP:CZ3	2.94	0.55
1:E:7:GLU:O	1:E:11:ARG:HG3	2.06	0.55
1:H:120:ARG:HH11	1:H:120:ARG:CB	2.14	0.55
1:H:293:TRP:O	1:H:299:VAL:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:394:ASP:O	1:H:398:ARG:HG3	2.07	0.55
1:F:63:ARG:HG3	1:F:69:TRP:CE2	2.42	0.54
1:F:548:LEU:HG	1:F:613:ILE:HB	1.89	0.54
1:H:571:VAL:CG2	1:H:617:GLU:HB3	2.38	0.54
1:F:198:TRP:CH2	1:F:427:VAL:HG21	2.42	0.54
1:B:267:HIS:CE1	1:B:269:ASP:HB2	2.41	0.54
1:H:571:VAL:HG21	1:H:617:GLU:HB3	1.89	0.54
1:H:17:PHE:H	1:H:284:ASN:HD21	1.55	0.54
1:H:105:PRO:HA	1:H:114:LEU:HA	1.89	0.54
1:C:174:ASP:OD1	1:C:228:ARG:NH2	2.34	0.54
1:E:522:TRP:CZ3	1:E:533:ILE:CD1	2.91	0.54
1:F:250:TYR:HA	1:F:258:GLU:OE2	2.06	0.54
1:H:426:VAL:HG13	1:H:432:SER:HA	1.89	0.54
1:A:174:ASP:OD1	1:A:228:ARG:NH2	2.40	0.54
1:G:395:PRO:HA	1:G:398:ARG:HD2	1.90	0.54
1:A:313:ARG:HG2	1:A:330:ASN:HB2	1.90	0.54
1:A:214:THR:HG23	1:A:215:PRO:HD2	1.90	0.53
1:A:330:ASN:O	1:A:334:ILE:HG13	2.08	0.53
1:C:582:SER:HB3	1:C:584:MET:HG3	1.89	0.53
1:C:3:TRP:HB2	1:C:34:TRP:CZ3	2.43	0.53
1:C:154:TRP:CD1	1:C:466:MET:HE2	2.43	0.53
1:D:11:ARG:NH2	1:D:19:ASP:OD1	2.41	0.53
1:F:63:ARG:HG3	1:F:69:TRP:CZ2	2.43	0.53
1:F:250:TYR:N	1:F:258:GLU:OE2	2.41	0.53
1:A:150:HIS:HA	2:A:708:HOH:O	2.08	0.53
1:D:20:SER:HB2	1:D:24:LEU:HD12	1.91	0.53
1:E:491:TYR:O	1:E:495:ILE:HD12	2.09	0.53
1:G:466:MET:HB3	1:G:482:LEU:HD11	1.90	0.53
1:C:575:ASP:OD1	1:C:582:SER:N	2.37	0.53
1:H:524:ASP:OD2	1:H:598:HIS:CD2	2.62	0.53
1:B:192:HIS:CG	1:B:199:GLY:HA2	2.44	0.53
1:F:218:LEU:HD23	1:F:297:TYR:CE2	2.44	0.53
1:H:565:GLY:HA2	1:H:592:ALA:HB3	1.90	0.53
1:E:201:GLN:C	1:E:242:ALA:HB2	2.34	0.53
1:F:175:TYR:O	1:F:179:LEU:HD12	2.09	0.53
1:B:107:THR:HG22	1:D:490:PRO:HB3	1.90	0.53
1:B:403:ASP:CG	1:B:528:ARG:HH22	2.16	0.53
1:G:258:GLU:CD	1:G:258:GLU:H	2.16	0.53
1:G:307:VAL:HG21	1:G:355:ALA:HB1	1.91	0.53
1:H:3:TRP:HB2	1:H:34:TRP:CZ3	2.44	0.53
1:A:97:ASP:HB3	1:A:100:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:564:ILE:HG22	1:F:568:TRP:HZ2	1.73	0.53
1:G:134:ARG:HH11	1:G:300:ASP:HA	1.72	0.53
1:A:574:SER:HB3	1:A:613:ILE:H	1.74	0.53
1:D:77:LEU:HB2	1:D:80:HIS:ND1	2.24	0.53
1:G:540:THR:HG22	1:G:541:ASP:N	2.21	0.53
1:E:152:GLY:HA3	1:E:195:TYR:OH	2.09	0.53
1:E:255:THR:HA	1:E:258:GLU:OE2	2.09	0.53
1:C:250:TYR:HE1	1:C:255:THR:HG22	1.72	0.52
1:H:390:TYR:HE2	1:H:550:PHE:CD2	2.27	0.52
1:B:436:LYS:NZ	2:B:701:HOH:O	2.27	0.52
1:C:473:HIS:NE2	1:C:492:HIS:HE1	2.07	0.52
1:G:150:HIS:ND1	1:G:153:SER:OG	2.34	0.52
1:A:244:ASP:HB3	1:A:247:GLY:H	1.73	0.52
1:D:570:GLU:HB2	1:D:588:GLY:H	1.73	0.52
1:H:169:ALA:HB1	1:H:224:TYR:HD2	1.74	0.52
1:A:214:THR:HG22	1:A:216:GLN:H	1.73	0.52
1:E:196:GLY:HA2	1:E:478:HIS:NE2	2.25	0.52
1:F:105:PRO:HA	1:F:114:LEU:H	1.74	0.52
1:B:395:PRO:HA	1:B:398:ARG:HG3	1.92	0.52
1:H:419:LEU:N	1:H:461:LYS:O	2.41	0.52
1:B:271:GLY:C	1:B:273:TYR:H	2.17	0.52
1:D:395:PRO:HB3	1:D:551:THR:HA	1.90	0.52
1:E:304:VAL:HG12	1:E:307:VAL:HG22	1.91	0.52
1:H:426:VAL:HG12	1:H:426:VAL:O	2.10	0.52
1:A:253:GLY:O	1:C:245:PRO:HG3	2.10	0.52
1:C:15:GLY:HA2	1:C:284:ASN:ND2	2.24	0.52
1:E:176:VAL:HG13	1:E:181:PHE:HB2	1.91	0.52
1:F:250:TYR:HA	1:F:254:THR:O	2.10	0.52
1:H:192:HIS:CG	1:H:199:GLY:HA2	2.45	0.52
1:H:573:ASN:HD21	1:H:585:GLY:HA2	1.75	0.52
1:C:103:MET:HB2	1:C:191:GLU:HG2	1.92	0.52
1:E:49:GLY:HA2	1:E:54:TRP:CZ3	2.45	0.52
1:E:95:LYS:NZ	1:E:245:PRO:O	2.43	0.52
1:G:456:TRP:HA	1:G:462:LYS:HD2	1.92	0.52
1:A:554:PRO:CB	1:A:584:MET:HE1	2.39	0.52
1:E:334:ILE:O	1:E:338:LYS:HG3	2.09	0.52
1:G:521:GLU:OE2	1:G:600:ARG:NH1	2.38	0.51
1:A:9:ILE:HG12	1:A:65:GLY:HA3	1.90	0.51
1:B:267:HIS:HB3	1:B:271:GLY:HA2	1.92	0.51
1:B:456:TRP:HA	1:B:462:LYS:CE	2.39	0.51
1:B:95:LYS:NZ	1:B:249:VAL:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:THR:HG22	1:B:481:GLN:H	1.75	0.51
1:E:307:VAL:HG21	1:E:355:ALA:HB1	1.92	0.51
1:G:18:TYR:HB3	1:G:291:LEU:HD12	1.92	0.51
1:A:7:GLU:O	1:A:11:ARG:HG3	2.09	0.51
1:A:178:ASP:O	1:A:500:ARG:HG3	2.11	0.51
1:C:405:LEU:HD21	1:C:533:ILE:HD13	1.93	0.51
1:F:154:TRP:HD1	1:F:466:MET:HE2	1.76	0.51
1:F:402:HIS:O	1:F:406:THR:HG23	2.10	0.51
1:D:278:ASN:ND2	1:D:332:GLU:HG2	2.25	0.51
1:H:498:TRP:CZ3	1:H:572:LEU:HD13	2.46	0.51
1:B:179:LEU:HD21	1:B:496:GLN:HG3	1.92	0.51
1:H:33:THR:HG23	1:H:76:ALA:O	2.10	0.51
1:A:197:SER:HB2	1:A:201:GLN:HG2	1.93	0.51
1:D:151:LEU:HD22	1:D:168:ILE:HD13	1.92	0.51
1:D:189:ILE:HD11	1:D:234:LEU:CD1	2.41	0.51
1:F:546:PHE:HD2	1:F:613:ILE:HD11	1.76	0.51
1:G:153:SER:CB	1:G:476:TRP:HE1	2.24	0.51
1:F:12:TRP:HD1	1:F:66:ALA:HB1	1.76	0.50
1:F:551:THR:HG22	1:F:553:VAL:N	2.24	0.50
1:H:125:TRP:CD1	1:H:298:HIS:HE2	2.30	0.50
1:D:559:ARG:HA	1:D:604:LEU:O	2.11	0.50
1:H:24:LEU:HA	1:H:36:CYS:HB3	1.93	0.50
1:A:4:LEU:HD12	1:A:64:TYR:HB2	1.94	0.50
1:B:534:CYS:HA	1:B:546:PHE:O	2.11	0.50
1:D:409:LEU:HD13	1:D:522:TRP:CZ2	2.45	0.50
1:F:352:ILE:HG23	1:F:376:LEU:HD23	1.92	0.50
1:A:192:HIS:CG	1:A:199:GLY:HA2	2.47	0.50
1:C:13:GLU:HG3	1:C:66:ALA:HB2	1.92	0.50
1:E:424:ASP:O	1:E:430:LYS:HE3	2.12	0.50
1:G:554:PRO:HB3	1:G:584:MET:HE1	1.93	0.50
1:H:41:HIS:HB2	1:H:252:ASP:OD2	2.12	0.50
1:B:456:TRP:HA	1:B:462:LYS:HE2	1.94	0.50
1:C:134:ARG:HD2	1:C:300:ASP:OD1	2.12	0.50
1:D:18:TYR:HB3	1:D:291:LEU:HD12	1.94	0.50
1:F:106:PRO:HD2	1:F:113:GLY:HA3	1.92	0.50
1:G:248:LEU:HB3	1:G:257:PHE:CD2	2.47	0.50
1:A:104:GLU:HB2	1:A:117:ILE:HD11	1.93	0.50
1:B:267:HIS:HB3	1:B:271:GLY:N	2.27	0.50
1:C:12:TRP:HZ2	1:C:38:TRP:CD2	2.30	0.50
1:C:473:HIS:NE2	1:C:492:HIS:CE1	2.80	0.50
1:E:250:TYR:HA	1:E:258:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:SER:HB3	1:F:167:GLU:HB2	1.93	0.50
1:F:460:GLY:H	1:F:515:ASP:CG	2.18	0.50
1:H:167:GLU:O	1:H:171:PRO:HD2	2.11	0.50
1:A:311:LEU:HD13	1:A:361:TRP:CD2	2.46	0.50
1:E:246:GLN:CD	1:E:246:GLN:H	2.19	0.50
1:H:189:ILE:HD12	1:H:190:MET:HG3	1.93	0.50
1:A:139:SER:HA	1:A:142:GLU:HG3	1.93	0.50
1:D:391:MET:HG3	1:D:451:LEU:HD12	1.94	0.50
1:E:120:ARG:HH11	1:E:120:ARG:HG3	1.77	0.50
1:E:136:GLY:HA2	1:E:352:ILE:HD11	1.92	0.50
1:B:47:VAL:CG2	1:B:61:LEU:HD21	2.42	0.49
1:D:77:LEU:HB2	1:D:80:HIS:CE1	2.47	0.49
1:H:37:VAL:HG11	1:H:45:VAL:HG11	1.94	0.49
1:H:391:MET:CE	1:H:451:LEU:HB2	2.41	0.49
1:H:521:GLU:HB3	1:H:536:LEU:HB3	1.94	0.49
1:C:61:LEU:HD22	1:C:71:GLY:HA3	1.93	0.49
1:A:95:LYS:HD2	1:A:246:GLN:O	2.13	0.49
1:B:395:PRO:HB3	1:B:551:THR:HA	1.94	0.49
1:D:3:TRP:HB2	1:D:34:TRP:CZ3	2.48	0.49
1:G:427:VAL:HG11	1:G:476:TRP:HE3	1.77	0.49
1:D:480:THR:OG1	1:D:481:GLN:N	2.45	0.49
1:E:135:LYS:HA	1:E:135:LYS:HE2	1.94	0.49
1:B:267:HIS:HB3	1:B:271:GLY:CA	2.43	0.49
1:C:5:THR:HG22	1:C:7:GLU:H	1.76	0.49
1:C:465:PHE:CE1	1:C:466:MET:HG2	2.47	0.49
1:F:154:TRP:CD1	1:F:466:MET:HE2	2.47	0.49
1:F:202:VAL:N	1:F:242:ALA:HB2	2.28	0.49
1:F:284:ASN:H	1:F:284:ASN:HD22	1.59	0.49
1:H:169:ALA:HB2	1:H:221:LEU:HD12	1.94	0.49
1:A:574:SER:HB2	1:A:613:ILE:HG23	1.94	0.49
1:D:214:THR:HG22	1:D:217:ASP:H	1.77	0.49
1:D:215:PRO:O	1:D:219:MET:HG3	2.12	0.49
1:E:175:TYR:OH	1:E:470:PHE:HE1	1.95	0.49
1:G:459:PRO:HA	1:G:537:ARG:NH2	2.28	0.49
1:B:103:MET:HB2	1:B:191:GLU:HG2	1.94	0.49
1:C:143:PRO:HD3	1:C:513:TRP:CE2	2.46	0.49
1:E:469:GLU:O	1:E:495:ILE:HG22	2.13	0.49
1:G:594:PRO:HA	1:G:602:PHE:HD1	1.77	0.49
1:A:527:ASP:OD1	1:A:530:GLN:HG3	2.12	0.49
1:B:153:SER:O	1:B:481:GLN:HA	2.12	0.49
1:C:395:PRO:HA	1:C:398:ARG:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ASP:OD2	1:B:22:ARG:NE	2.45	0.49
1:B:140:LEU:HD21	1:B:416:HIS:CG	2.48	0.49
1:E:278:ASN:OD1	1:E:332:GLU:HG2	2.13	0.49
1:G:143:PRO:HD3	1:G:513:TRP:CE2	2.47	0.49
1:H:291:LEU:O	1:H:295:ASP:N	2.43	0.49
1:H:294:LEU:HD23	1:H:299:VAL:HG23	1.95	0.49
1:A:37:VAL:HG22	1:A:84:TYR:CZ	2.48	0.49
1:B:355:ALA:HB2	1:B:375:PHE:CD2	2.48	0.49
1:D:130:TRP:HD1	1:D:131:MET:HG3	1.78	0.49
1:E:49:GLY:HA3	1:E:51:PHE:CE1	2.48	0.49
1:E:395:PRO:HA	1:E:398:ARG:HD2	1.95	0.49
1:G:378:LYS:HD3	1:G:417:TYR:CE1	2.44	0.49
1:H:351:ALA:C	1:H:352:ILE:HG13	2.38	0.49
1:B:148:GLU:HB2	1:B:463:LEU:HD21	1.95	0.48
1:C:307:VAL:HG21	1:C:355:ALA:HB1	1.95	0.48
1:F:399:LYS:HD2	1:F:400:TYR:CZ	2.47	0.48
1:F:406:THR:HG22	1:F:533:ILE:HD11	1.94	0.48
1:G:187:LEU:HD23	1:G:200:TYR:HE2	1.78	0.48
1:H:469:GLU:H	1:H:469:GLU:CD	2.11	0.48
1:E:245:PRO:HG2	1:E:246:GLN:NE2	2.28	0.48
1:E:522:TRP:CH2	1:E:533:ILE:CD1	2.96	0.48
1:H:270:TRP:HD1	1:H:274:VAL:HG22	1.78	0.48
1:A:453:GLY:HA3	1:A:613:ILE:HG21	1.94	0.48
1:D:406:THR:HG22	1:D:533:ILE:HD11	1.95	0.48
1:E:544:LEU:HD22	1:E:615:ILE:HG22	1.94	0.48
1:G:8:ASP:O	1:G:9:ILE:C	2.56	0.48
1:H:61:LEU:HD22	1:H:71:GLY:HA3	1.95	0.48
1:H:365:SER:OG	1:H:415:GLU:HB3	2.13	0.48
1:B:165:TYR:CZ	1:B:212:TYR:HB2	2.49	0.48
1:B:431:GLY:O	1:B:436:LYS:HE2	2.13	0.48
1:B:461:LYS:C	1:B:462:LYS:HD3	2.38	0.48
1:C:394:ASP:OD1	1:C:396:VAL:HG22	2.14	0.48
1:D:584:MET:HG3	1:D:610:PRO:HD3	1.95	0.48
1:G:331:LEU:O	1:G:332:GLU:C	2.55	0.48
1:G:596:SER:O	1:G:597:TRP:HE3	1.95	0.48
1:H:601:PRO:HB2	1:H:602:PHE:CD1	2.49	0.48
1:E:440:ASP:OD2	1:E:440:ASP:C	2.56	0.48
1:H:35:PHE:HZ	1:H:118:ILE:HD11	1.79	0.48
1:G:17:PHE:CE1	1:G:19:ASP:HB2	2.41	0.48
1:H:267:HIS:ND1	1:H:268:PRO:HD2	2.29	0.48
1:A:270:TRP:HD1	1:A:274:VAL:HG22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:HIS:HB3	1:H:31:GLU:OE2	2.14	0.48
1:D:457:GLY:O	1:D:537:ARG:HD2	2.13	0.48
1:E:437:MET:HE3	1:E:448:LEU:HD12	1.95	0.48
1:G:3:TRP:O	1:G:23:LYS:HE2	2.14	0.48
1:H:125:TRP:CD2	1:H:298:HIS:CD2	3.01	0.48
1:A:151:LEU:HD22	1:A:168:ILE:HD13	1.94	0.48
1:A:163:PHE:HD1	1:A:167:GLU:HB3	1.79	0.48
1:A:424:ASP:HB2	2:A:715:HOH:O	2.13	0.48
1:A:506:TYR:HA	1:A:512:LEU:HD12	1.96	0.48
1:C:473:HIS:HB2	1:C:474:HIS:CD2	2.48	0.48
1:D:96:THR:HG22	1:D:246:GLN:O	2.14	0.48
1:B:59:HIS:CG	1:B:73:VAL:HG22	2.49	0.48
1:C:35:PHE:CE2	1:C:47:VAL:HG11	2.49	0.48
1:C:193:PRO:HG3	1:C:203:VAL:HG21	1.96	0.48
1:C:392:ARG:HG2	1:C:392:ARG:HH11	1.78	0.48
1:C:418:ILE:HG12	1:C:461:LYS:HB2	1.96	0.48
1:C:511:ALA:HB1	1:C:537:ARG:O	2.14	0.48
1:D:15:GLY:HA2	1:D:284:ASN:ND2	2.28	0.48
1:D:449:ARG:HG3	1:D:495:ILE:HG12	1.96	0.48
1:F:90:PHE:HB3	1:F:91:TYR:CE2	2.49	0.48
1:A:111:ILE:HD12	1:A:111:ILE:H	1.79	0.47
1:E:99:TYR:CE1	1:E:285:PHE:HD1	2.32	0.47
1:F:249:VAL:HG12	1:F:250:TYR:CD2	2.49	0.47
1:H:293:TRP:C	1:H:299:VAL:HG22	2.39	0.47
1:H:472:GLN:HE22	1:H:482:LEU:HD22	1.78	0.47
1:C:56:PRO:HB3	1:C:85:ARG:HD2	1.94	0.47
1:C:131:MET:HE1	1:C:134:ARG:NH1	2.29	0.47
1:E:245:PRO:HG2	1:E:246:GLN:HE21	1.78	0.47
1:F:7:GLU:O	1:F:11:ARG:HG3	2.15	0.47
1:A:3:TRP:O	1:A:23:LYS:NZ	2.40	0.47
1:A:568:TRP:HB2	1:A:590:VAL:HG13	1.94	0.47
1:B:62:GLU:HB3	1:B:64:TYR:HE2	1.78	0.47
1:C:7:GLU:O	1:C:11:ARG:HG3	2.14	0.47
1:G:442:TRP:CE3	1:G:443:GLN:HG3	2.44	0.47
1:A:157:LYS:HD3	1:A:167:GLU:OE1	2.14	0.47
1:A:562:VAL:HG11	1:A:604:LEU:HG	1.96	0.47
1:C:552:PRO:O	1:C:610:PRO:HB3	2.15	0.47
1:D:331:LEU:H	1:D:331:LEU:HD12	1.79	0.47
1:E:559:ARG:HA	1:E:604:LEU:O	2.15	0.47
1:H:574:SER:HB2	1:H:613:ILE:HG22	1.96	0.47
1:G:255:THR:HA	1:G:258:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:ASN:OD1	1:C:614:LEU:HD22	2.15	0.47
1:D:523:ILE:HD11	1:D:536:LEU:HD13	1.95	0.47
1:E:545:LEU:HD12	1:E:546:PHE:N	2.29	0.47
1:H:246:GLN:H	1:H:246:GLN:HG3	1.33	0.47
1:H:423:HIS:HB3	1:H:465:PHE:CE1	2.50	0.47
1:A:419:LEU:N	1:A:461:LYS:O	2.42	0.47
1:D:153:SER:CB	1:D:476:TRP:HE1	2.28	0.47
1:D:157:LYS:HG2	1:D:163:PHE:CE1	2.50	0.47
1:D:540:THR:OG1	1:D:541:ASP:N	2.44	0.47
1:E:51:PHE:CD2	1:E:73:VAL:HG11	2.50	0.47
1:E:440:ASP:OD2	1:E:443:GLN:HG3	2.15	0.47
1:G:313:ARG:NH1	1:G:332:GLU:OE2	2.46	0.47
1:H:192:HIS:CD2	1:H:211:ARG:HH21	2.32	0.47
1:H:245:PRO:C	1:H:247:GLY:N	2.70	0.47
1:H:391:MET:HE2	1:H:451:LEU:HB2	1.95	0.47
1:F:271:GLY:O	1:F:272:THR:HB	2.14	0.47
1:B:424:ASP:O	1:B:430:LYS:HE3	2.14	0.47
1:C:36:CYS:HA	1:C:69:TRP:O	2.15	0.47
1:C:250:TYR:HE1	1:C:255:THR:CG2	2.28	0.47
1:E:522:TRP:CZ3	1:E:533:ILE:HD11	2.50	0.47
1:F:214:THR:HG22	1:F:215:PRO:HD2	1.97	0.47
1:G:134:ARG:NH1	1:G:300:ASP:HA	2.28	0.47
1:A:196:GLY:HA2	1:A:478:HIS:CD2	2.50	0.47
1:C:5:THR:O	1:C:8:ASP:HB2	2.14	0.47
1:C:97:ASP:HB3	1:C:100:ALA:HB2	1.97	0.47
1:C:334:ILE:O	1:C:338:LYS:HG3	2.15	0.47
1:D:131:MET:SD	1:D:298:HIS:HB3	2.54	0.47
1:F:105:PRO:HG3	1:F:210:PHE:CZ	2.50	0.47
1:A:278:ASN:CG	1:A:332:GLU:HG2	2.39	0.46
1:B:380:ASN:HB2	1:B:417:TYR:HB3	1.96	0.46
1:D:97:ASP:HB3	1:D:100:ALA:HB2	1.97	0.46
1:D:267:HIS:CG	1:D:268:PRO:HD2	2.50	0.46
1:F:222:ILE:HG21	1:F:297:TYR:O	2.15	0.46
1:G:96:THR:HG22	1:G:246:GLN:O	2.15	0.46
1:H:437:MET:HG3	1:H:447:ASN:HB2	1.97	0.46
1:G:474:HIS:ND1	1:G:475:GLU:N	2.63	0.46
1:G:484:TRP:O	1:G:487:LEU:HB2	2.14	0.46
1:H:235:ASP:OD1	1:H:303:ARG:HD3	2.15	0.46
1:E:153:SER:CB	1:E:476:TRP:HE1	2.29	0.46
1:F:355:ALA:HB2	1:F:375:PHE:CD2	2.51	0.46
1:H:17:PHE:H	1:H:284:ASN:ND2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:PRO:HA	1:A:67:GLY:HA2	1.98	0.46
1:B:170:GLU:HB3	1:B:171:PRO:HD3	1.98	0.46
1:B:403:ASP:OD2	1:F:329:GLU:OE2	2.33	0.46
1:C:267:HIS:O	1:C:271:GLY:N	2.48	0.46
1:H:560:VAL:HA	1:H:598:HIS:CE1	2.51	0.46
1:A:366:ALA:HB3	1:A:372:GLY:HA3	1.98	0.46
1:H:153:SER:CB	1:H:476:TRP:HE1	2.29	0.46
1:B:489:GLN:HB2	1:B:492:HIS:HD2	1.81	0.46
1:D:510:PRO:HA	1:D:513:TRP:CG	2.51	0.46
1:E:61:LEU:N	1:E:61:LEU:HD23	2.31	0.46
1:F:97:ASP:HB3	1:F:100:ALA:HB2	1.97	0.46
1:F:433:LEU:HA	1:F:436:LYS:HD2	1.98	0.46
1:G:62:GLU:HG3	1:G:64:TYR:CE1	2.46	0.46
1:B:53:ASN:HA	1:D:584:MET:HE1	1.98	0.46
1:E:236:TRP:HB2	1:E:302:LEU:HD22	1.97	0.46
1:F:190:MET:HE1	1:F:235:ASP:O	2.16	0.46
1:D:165:TYR:O	1:D:168:ILE:HG22	2.16	0.46
1:F:153:SER:CB	1:F:476:TRP:HE1	2.29	0.46
1:F:277:TYR:OH	1:F:310:MET:HE3	2.16	0.46
1:A:391:MET:HE2	1:A:451:LEU:HB2	1.98	0.46
1:C:12:TRP:CE2	1:C:68:LEU:HD21	2.51	0.46
1:E:35:PHE:CE2	1:E:47:VAL:HG11	2.51	0.46
1:E:381:MET:HB3	1:E:381:MET:HE3	1.66	0.46
1:H:426:VAL:HG12	1:H:476:TRP:H	1.80	0.46
1:H:573:ASN:HB3	1:H:576:ALA:HB2	1.98	0.46
1:C:49:GLY:HA2	1:C:54:TRP:CZ3	2.51	0.45
1:F:391:MET:O	1:F:438:PRO:HD3	2.16	0.45
1:G:12:TRP:HA	1:G:284:ASN:ND2	2.31	0.45
1:H:103:MET:HB3	1:H:114:LEU:HD22	1.97	0.45
1:H:125:TRP:CG	1:H:298:HIS:HE2	2.34	0.45
1:A:312:TYR:OH	1:A:359:THR:HG21	2.16	0.45
1:C:20:SER:HB2	1:C:24:LEU:CD1	2.46	0.45
1:C:105:PRO:HB3	1:C:113:GLY:O	2.16	0.45
1:C:128:ASP:O	1:C:132:GLN:HG3	2.17	0.45
1:D:258:GLU:O	1:D:279:LYS:NZ	2.49	0.45
1:D:419:LEU:HD11	1:D:458:HIS:HB3	1.97	0.45
1:E:534:CYS:HA	1:E:546:PHE:O	2.16	0.45
1:F:472:GLN:HG2	1:F:473:HIS:N	2.30	0.45
1:G:29:ASP:OD1	1:G:72:TYR:CE1	2.67	0.45
1:B:28:PRO:HG3	1:B:118:ILE:CG2	2.47	0.45
1:D:123:TYR:OH	1:D:220:TYR:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:MET:HE1	1:A:235:ASP:O	2.17	0.45
1:A:523:ILE:HB	1:A:534:CYS:HB2	1.99	0.45
1:B:437:MET:CE	1:B:447:ASN:HB3	2.43	0.45
1:C:469:GLU:O	1:C:495:ILE:HG22	2.17	0.45
1:D:192:HIS:CG	1:D:199:GLY:HA2	2.51	0.45
1:E:312:TYR:HE2	1:E:359:THR:HG21	1.81	0.45
1:F:201:GLN:C	1:F:242:ALA:HB2	2.42	0.45
1:A:165:TYR:HB2	1:A:217:ASP:HB3	1.99	0.45
1:A:173:ALA:O	1:A:177:GLN:HG3	2.15	0.45
1:A:480:THR:HG22	1:A:481:GLN:O	2.17	0.45
1:B:2:SER:OG	1:B:3:TRP:N	2.47	0.45
1:C:574:SER:HB3	1:C:613:ILE:HG23	1.97	0.45
1:E:166:ARG:HD2	1:E:220:TYR:CD2	2.52	0.45
1:F:48:LEU:HD12	1:F:83:LYS:HD3	1.97	0.45
1:F:189:ILE:HD12	1:F:218:LEU:HD21	1.97	0.45
1:F:345:TYR:OH	1:F:376:LEU:HB2	2.16	0.45
1:F:448:LEU:HD23	1:F:448:LEU:HA	1.76	0.45
1:H:419:LEU:HD11	1:H:458:HIS:HB3	1.98	0.45
1:B:17:PHE:N	1:B:284:ASN:OD1	2.49	0.45
1:E:191:GLU:OE2	1:E:210:PHE:HD1	1.99	0.45
1:E:423:HIS:HB2	1:E:476:TRP:CE3	2.52	0.45
1:E:426:VAL:O	1:E:475:GLU:HB3	2.17	0.45
1:H:391:MET:SD	1:H:550:PHE:HE2	2.39	0.45
1:A:83:LYS:HD2	1:A:94:ASP:HB3	1.99	0.45
1:A:191:GLU:OE2	1:A:209:THR:HA	2.16	0.45
1:A:610:PRO:O	1:A:611:LEU:C	2.59	0.45
1:B:536:LEU:HD21	1:B:563:PRO:HG2	1.99	0.45
1:B:601:PRO:HB2	1:B:602:PHE:CD1	2.52	0.45
1:F:196:GLY:HA2	1:F:478:HIS:NE2	2.31	0.45
1:H:145:SER:N	1:H:182:THR:HG22	2.20	0.45
1:H:418:ILE:HG12	1:H:461:LYS:HB2	1.99	0.45
1:A:355:ALA:HB2	1:A:375:PHE:CE1	2.52	0.45
1:D:40:PRO:O	1:D:63:ARG:NH2	2.49	0.45
1:H:551:THR:OG1	1:H:552:PRO:HD2	2.16	0.45
1:A:18:TYR:HB3	1:A:291:LEU:HD12	1.98	0.45
1:C:559:ARG:HA	1:C:604:LEU:O	2.16	0.45
1:D:433:LEU:HB3	1:D:448:LEU:HD11	1.99	0.45
1:D:570:GLU:H	1:D:588:GLY:HA2	1.82	0.45
1:F:608:LEU:HA	1:F:609:PRO:HD3	1.79	0.45
1:H:487:LEU:HA	1:H:487:LEU:HD23	1.67	0.45
1:C:345:TYR:OH	1:C:376:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:MET:HE3	1:C:381:MET:HB3	1.75	0.45
1:E:278:ASN:CG	1:E:332:GLU:HG2	2.42	0.45
1:F:82:TYR:CE1	1:F:116:SER:HB3	2.51	0.45
1:F:250:TYR:CA	1:F:258:GLU:OE2	2.65	0.45
1:A:532:VAL:HG13	1:A:548:LEU:O	2.17	0.44
1:D:48:LEU:HD13	1:D:54:TRP:O	2.16	0.44
1:D:234:LEU:CD1	1:D:299:VAL:HG21	2.47	0.44
1:A:153:SER:CB	1:A:476:TRP:HE1	2.29	0.44
1:D:330:ASN:O	1:D:334:ILE:HG13	2.17	0.44
1:G:391:MET:HE3	1:G:391:MET:HB3	1.86	0.44
1:A:185:GLU:HG3	1:A:233:ILE:HB	1.99	0.44
1:D:179:LEU:HD11	1:D:469:GLU:HG3	2.00	0.44
1:E:474:HIS:NE2	1:E:483:GLU:OE2	2.51	0.44
1:A:12:TRP:HA	1:A:284:ASN:ND2	2.33	0.44
1:B:107:THR:CG2	1:D:490:PRO:HB3	2.46	0.44
1:B:523:ILE:HD11	1:B:536:LEU:HB2	2.00	0.44
1:C:431:GLY:O	1:C:436:LYS:HE2	2.17	0.44
1:F:510:PRO:HA	1:F:513:TRP:CG	2.52	0.44
1:G:154:TRP:HE3	1:G:168:ILE:HD11	1.82	0.44
1:G:449:ARG:HD2	1:G:579:TYR:HB3	1.99	0.44
1:G:465:PHE:CE1	1:G:466:MET:HG3	2.52	0.44
1:G:546:PHE:HB3	1:G:548:LEU:HD11	1.99	0.44
1:H:154:TRP:CZ3	1:H:155:ARG:HD2	2.53	0.44
1:H:189:ILE:HD12	1:H:190:MET:N	2.33	0.44
1:H:472:GLN:HG3	1:H:483:GLU:HG3	1.98	0.44
1:B:12:TRP:HA	1:B:284:ASN:HD21	1.83	0.44
1:C:35:PHE:O	1:C:70:ALA:HA	2.16	0.44
1:C:592:ALA:HA	1:C:604:LEU:HD23	1.98	0.44
1:F:28:PRO:HG3	1:F:118:ILE:HG23	1.99	0.44
1:H:256:LEU:O	1:H:279:LYS:NZ	2.45	0.44
1:H:521:GLU:OE1	1:H:600:ARG:NH1	2.37	0.44
1:A:538:LYS:HE3	1:A:538:LYS:HB2	1.88	0.44
1:C:510:PRO:HA	1:C:513:TRP:CD2	2.52	0.44
1:E:82:TYR:OH	1:E:97:ASP:OD2	2.27	0.44
1:E:330:ASN:OD1	1:E:332:GLU:HB2	2.17	0.44
1:E:534:CYS:SG	1:E:547:VAL:HG13	2.58	0.44
1:F:241:PHE:HE1	1:F:249:VAL:HG22	1.83	0.44
1:F:484:TRP:O	1:F:487:LEU:HB2	2.16	0.44
1:G:83:LYS:HD2	1:G:94:ASP:CG	2.41	0.44
1:C:601:PRO:HB2	1:C:602:PHE:CD1	2.52	0.44
1:D:103:MET:O	1:D:210:PHE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:507:ARG:NH2	2:E:703:HOH:O	2.51	0.44
1:G:35:PHE:HZ	1:G:118:ILE:HD11	1.83	0.44
1:H:103:MET:HE3	1:H:103:MET:HB2	1.70	0.44
1:D:381:MET:HE3	1:D:381:MET:HB3	1.87	0.44
1:D:432:SER:O	1:D:436:LYS:HG3	2.18	0.44
1:D:604:LEU:HD23	1:D:606:LEU:HD21	2.00	0.44
1:E:610:PRO:O	1:E:611:LEU:C	2.60	0.44
1:A:49:GLY:HA2	1:A:54:TRP:CZ3	2.53	0.44
1:A:181:PHE:C	1:A:507:ARG:HH21	2.25	0.44
1:B:88:HIS:CE1	1:B:254:THR:HG22	2.53	0.44
1:D:378:LYS:HD3	1:D:417:TYR:CE1	2.53	0.44
1:D:425:GLU:O	1:D:436:LYS:NZ	2.50	0.44
1:E:244:ASP:OD1	1:E:245:PRO:HD2	2.17	0.44
1:G:28:PRO:HG3	1:G:118:ILE:HG22	2.00	0.44
1:G:482:LEU:O	1:G:484:TRP:CD1	2.70	0.44
1:B:459:PRO:HA	1:B:537:ARG:NH2	2.32	0.43
1:F:364:VAL:HG13	1:F:373:LEU:HD12	1.99	0.43
1:A:391:MET:HE3	1:A:391:MET:HB3	1.80	0.43
1:A:568:TRP:CD1	1:A:604:LEU:HD21	2.53	0.43
1:B:154:TRP:CD1	1:B:466:MET:HE2	2.51	0.43
1:D:35:PHE:CD2	1:D:47:VAL:HG21	2.53	0.43
1:D:47:VAL:C	1:D:48:LEU:HD23	2.42	0.43
1:D:151:LEU:HD22	1:D:168:ILE:CD1	2.48	0.43
1:E:135:LYS:HD3	1:E:138:ALA:HB3	1.99	0.43
1:E:270:TRP:HD1	1:E:274:VAL:HG22	1.83	0.43
1:E:522:TRP:HH2	1:E:533:ILE:HD11	1.80	0.43
1:G:544:LEU:HB3	1:G:546:PHE:HE1	1.83	0.43
1:H:29:ASP:OD1	1:H:31:GLU:N	2.48	0.43
1:H:154:TRP:CD1	1:H:466:MET:CE	3.01	0.43
1:H:568:TRP:CZ3	1:H:618:PRO:HD3	2.53	0.43
1:C:548:LEU:HG	1:C:613:ILE:HD12	1.99	0.43
1:D:136:GLY:H	1:D:139:SER:HB3	1.82	0.43
1:E:453:GLY:HA3	1:E:613:ILE:HG21	2.00	0.43
1:G:49:GLY:HA2	1:G:54:TRP:CZ3	2.54	0.43
1:G:332:GLU:H	1:G:332:GLU:HG3	1.09	0.43
1:G:421:LEU:HD13	1:G:433:LEU:HD11	2.00	0.43
1:G:534:CYS:HA	1:G:546:PHE:O	2.18	0.43
1:H:536:LEU:HG	1:H:543:LEU:HD22	1.99	0.43
1:A:137:PRO:HD3	1:A:350:GLU:HA	1.99	0.43
1:A:141:TYR:O	1:A:513:TRP:HB3	2.18	0.43
1:B:19:ASP:OD1	1:B:19:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:SER:OG	1:D:163:PHE:N	2.52	0.43
1:D:584:MET:H	1:D:584:MET:HG2	1.45	0.43
1:F:113:GLY:O	1:F:114:LEU:HB2	2.19	0.43
1:F:596:SER:HA	1:F:600:ARG:O	2.19	0.43
1:G:547:VAL:C	1:G:548:LEU:HD12	2.43	0.43
1:H:151:LEU:HD11	1:H:186:LEU:HD13	1.99	0.43
1:H:193:PRO:HD3	1:H:203:VAL:CG1	2.46	0.43
1:H:461:LYS:C	1:H:462:LYS:HD2	2.43	0.43
1:D:59:HIS:CD2	1:D:73:VAL:HG22	2.54	0.43
1:D:564:ILE:HG22	1:D:565:GLY:O	2.17	0.43
1:E:431:GLY:N	1:E:475:GLU:OE1	2.52	0.43
1:G:331:LEU:HD13	1:G:331:LEU:HA	1.75	0.43
1:A:123:TYR:OH	1:A:220:TYR:HA	2.18	0.43
1:A:549:ASN:OD1	1:A:551:THR:HG22	2.18	0.43
1:B:48:LEU:HD11	1:B:56:PRO:HA	1.99	0.43
1:C:278:ASN:O	1:C:283:ARG:NH2	2.49	0.43
1:C:575:ASP:OD2	1:C:582:SER:HB2	2.18	0.43
1:D:104:GLU:CD	1:D:117:ILE:HD12	2.44	0.43
1:D:276:ASP:OD1	1:D:278:ASN:HB2	2.19	0.43
1:D:437:MET:O	1:D:444:LYS:NZ	2.42	0.43
1:E:95:LYS:HA	1:E:95:LYS:HD2	1.90	0.43
1:F:149:VAL:O	1:F:186:LEU:HA	2.19	0.43
1:F:403:ASP:O	1:F:407:PHE:HB2	2.19	0.43
1:F:552:PRO:O	1:F:610:PRO:HB3	2.18	0.43
1:G:149:VAL:HA	1:G:466:MET:CG	2.48	0.43
1:A:183:HIS:ND1	1:A:231:GLY:HA3	2.34	0.43
1:B:148:GLU:HB3	1:B:465:PHE:HA	2.01	0.43
1:C:101:PHE:HB2	1:C:119:THR:CG2	2.48	0.43
1:C:559:ARG:HD3	1:C:603:HIS:CE1	2.54	0.43
1:G:111:ILE:H	1:G:111:ILE:HG13	1.50	0.43
1:G:235:ASP:OD1	1:G:303:ARG:HD3	2.17	0.43
1:H:24:LEU:O	1:H:27:HIS:NE2	2.51	0.43
1:H:545:LEU:HB3	1:H:616:LEU:HB2	2.00	0.43
1:H:575:ASP:OD2	1:H:582:SER:N	2.52	0.43
1:B:552:PRO:O	1:B:610:PRO:HB3	2.17	0.43
1:C:155:ARG:HG2	1:C:484:TRP:HE1	1.82	0.43
1:F:244:ASP:OD2	1:F:244:ASP:C	2.62	0.43
1:F:562:VAL:HG21	1:F:604:LEU:HG	2.01	0.43
1:G:8:ASP:O	1:G:11:ARG:N	2.52	0.43
1:H:565:GLY:HA2	1:H:592:ALA:CB	2.49	0.43
1:B:364:VAL:HA	1:B:373:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:ALA:HB1	1:B:602:PHE:HB3	1.99	0.43
1:E:405:LEU:HD21	1:E:533:ILE:HG21	2.00	0.43
1:H:177:GLN:HG3	1:H:230:ILE:HD11	2.00	0.43
1:H:234:LEU:HG	1:H:299:VAL:HG11	2.01	0.43
1:A:354:ILE:HG12	1:A:377:TYR:HB2	2.00	0.43
1:A:396:VAL:O	1:A:399:LYS:HE2	2.19	0.43
1:B:567:PRO:HG2	1:B:619:GLU:HB3	1.99	0.43
1:C:576:ALA:HB3	1:C:579:TYR:CD2	2.54	0.43
1:C:593:VAL:O	1:C:595:GLU:N	2.44	0.43
1:E:255:THR:HG22	1:E:258:GLU:HG3	2.01	0.43
1:G:256:LEU:HD12	1:G:256:LEU:HA	1.88	0.43
1:G:571:VAL:HG21	1:G:617:GLU:HB3	2.01	0.43
1:H:85:ARG:NE	1:H:94:ASP:OD1	2.51	0.43
1:H:165:TYR:CE1	1:H:212:TYR:HB2	2.54	0.43
1:H:392:ARG:HD2	2:H:709:HOH:O	2.19	0.43
1:H:460:GLY:H	1:H:515:ASP:CG	2.26	0.43
1:A:524:ASP:OD2	1:A:598:HIS:NE2	2.52	0.42
1:D:9:ILE:HG21	1:D:65:GLY:HA3	2.01	0.42
1:D:491:TYR:HD1	1:D:491:TYR:HA	1.72	0.42
1:F:254:THR:HG22	1:F:255:THR:N	2.34	0.42
1:G:143:PRO:HD3	1:G:513:TRP:CD2	2.54	0.42
1:H:222:ILE:HG12	1:H:232:VAL:HG21	2.01	0.42
1:H:241:PHE:HB3	1:H:275:PHE:CZ	2.53	0.42
1:B:391:MET:CE	1:B:437:MET:HE1	2.48	0.42
1:B:392:ARG:NH2	1:B:430:LYS:O	2.52	0.42
1:B:544:LEU:HD23	1:B:544:LEU:HA	1.87	0.42
1:C:197:SER:HB2	1:C:201:GLN:HG2	2.00	0.42
1:F:96:THR:HG23	1:F:246:GLN:O	2.18	0.42
1:F:144:VAL:HB	1:F:461:LYS:HD2	2.00	0.42
1:F:514:HIS:O	1:F:537:ARG:NH1	2.48	0.42
1:H:29:ASP:OD1	1:H:29:ASP:C	2.63	0.42
1:A:19:ASP:CB	1:A:22:ARG:HD3	2.45	0.42
1:B:381:MET:HE3	1:B:381:MET:HB3	1.79	0.42
1:B:390:TYR:CE1	1:B:398:ARG:HB3	2.53	0.42
1:F:521:GLU:O	1:F:536:LEU:N	2.44	0.42
1:F:609:PRO:HA	1:F:610:PRO:HD3	1.92	0.42
1:B:28:PRO:HG3	1:B:118:ILE:HG23	2.00	0.42
1:B:146:ILE:HG21	1:B:185:GLU:HB2	2.02	0.42
1:B:241:PHE:CD2	1:B:248:LEU:HB2	2.54	0.42
1:C:49:GLY:HA3	1:C:51:PHE:CE2	2.54	0.42
1:F:538:LYS:O	1:F:538:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:165:TYR:CE2	1:H:218:LEU:HB2	2.55	0.42
1:H:256:LEU:HD12	1:H:256:LEU:HA	1.83	0.42
1:A:383:TRP:O	1:A:387:THR:OG1	2.34	0.42
1:A:505:LEU:HD12	1:A:509:HIS:CE1	2.54	0.42
1:C:114:LEU:HD12	1:C:114:LEU:HA	1.83	0.42
1:C:545:LEU:O	1:C:615:ILE:HA	2.19	0.42
1:C:593:VAL:C	1:C:595:GLU:H	2.24	0.42
1:F:557:HIS:HA	1:F:605:GLU:HG3	2.02	0.42
1:G:191:GLU:OE1	1:G:209:THR:HA	2.20	0.42
1:G:399:LYS:HG3	1:G:529:ASP:HA	2.01	0.42
1:H:3:TRP:CD1	1:H:4:LEU:CD1	3.02	0.42
1:A:261:ASP:HA	1:A:262:PRO:HD3	1.94	0.42
1:A:409:LEU:HD13	1:A:409:LEU:HA	1.87	0.42
1:B:194:TYR:CZ	1:B:196:GLY:HA3	2.55	0.42
1:B:252:ASP:OD1	1:B:252:ASP:N	2.45	0.42
1:B:267:HIS:HB3	1:B:271:GLY:H	1.85	0.42
1:C:131:MET:SD	1:C:134:ARG:HD3	2.60	0.42
1:C:562:VAL:CG2	1:C:602:PHE:HB2	2.48	0.42
1:D:286:LEU:HD23	1:D:286:LEU:HA	1.83	0.42
1:E:175:TYR:OH	1:E:470:PHE:CE1	2.72	0.42
1:G:250:TYR:HA	1:G:254:THR:O	2.19	0.42
1:H:245:PRO:C	1:H:247:GLY:H	2.27	0.42
1:H:449:ARG:O	1:H:498:TRP:NE1	2.52	0.42
1:B:114:LEU:HD12	1:B:114:LEU:HA	1.83	0.42
1:B:460:GLY:H	1:B:515:ASP:CG	2.27	0.42
1:D:136:GLY:HA2	1:D:352:ILE:HG12	2.02	0.42
1:F:35:PHE:O	1:F:70:ALA:HA	2.20	0.42
1:F:487:LEU:HD22	1:F:493:ARG:CZ	2.50	0.42
1:A:248:LEU:HD22	1:A:248:LEU:HA	1.86	0.42
1:B:246:GLN:CD	1:B:246:GLN:H	2.27	0.42
1:B:355:ALA:HB2	1:B:375:PHE:CE2	2.54	0.42
1:C:140:LEU:HD21	1:C:416:HIS:HB3	2.01	0.42
1:C:178:ASP:O	1:C:500:ARG:HG3	2.20	0.42
1:F:3:TRP:HB2	1:F:34:TRP:CZ3	2.55	0.42
1:F:192:HIS:CD2	1:F:199:GLY:HA2	2.54	0.42
1:G:36:CYS:HA	1:G:69:TRP:O	2.19	0.42
1:G:170:GLU:HB3	1:G:171:PRO:HD3	2.02	0.42
1:A:460:GLY:H	1:A:515:ASP:CG	2.27	0.42
1:C:179:LEU:HD21	1:C:496:GLN:HG2	2.01	0.42
1:F:157:LYS:HB2	1:F:157:LYS:HE3	1.93	0.42
1:G:466:MET:CB	1:G:482:LEU:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:PRO:HB3	1:C:297:TYR:OH	2.20	0.42
1:D:165:TYR:CZ	1:D:212:TYR:HB2	2.55	0.42
1:D:241:PHE:HZ	1:D:258:GLU:HG3	1.85	0.42
1:D:301:GLY:HA2	1:D:352:ILE:O	2.20	0.42
1:D:481:GLN:HG2	1:D:482:LEU:N	2.35	0.42
1:D:538:LYS:HB2	1:D:538:LYS:HE3	1.48	0.42
1:E:82:TYR:CD2	1:E:118:ILE:HG12	2.55	0.42
1:F:278:ASN:OD1	1:F:332:GLU:HB3	2.19	0.42
1:F:503:ASN:O	1:F:507:ARG:HG3	2.19	0.42
1:H:165:TYR:O	1:H:221:LEU:HD13	2.20	0.42
1:H:165:TYR:CZ	1:H:212:TYR:HB2	2.54	0.42
1:H:355:ALA:HB2	1:H:375:PHE:CG	2.55	0.42
1:A:154:TRP:CE3	1:A:155:ARG:HG3	2.55	0.41
1:A:165:TYR:CE2	1:A:212:TYR:HB2	2.55	0.41
1:B:406:THR:HG22	1:B:533:ILE:HD11	2.02	0.41
1:C:596:SER:HA	1:C:600:ARG:O	2.20	0.41
1:G:258:GLU:OE2	1:G:258:GLU:N	2.50	0.41
1:H:238:PRO:HG2	1:H:310:MET:HE1	2.01	0.41
1:A:90:PHE:CD2	1:C:83:LYS:HD3	2.55	0.41
1:A:94:ASP:HB3	1:C:91:TYR:HD1	1.86	0.41
1:B:21:TYR:O	1:B:27:HIS:NE2	2.49	0.41
1:B:215:PRO:HB3	1:B:297:TYR:OH	2.20	0.41
1:C:96:THR:HG22	1:C:246:GLN:O	2.20	0.41
1:D:378:LYS:HD3	1:D:417:TYR:HE1	1.84	0.41
1:D:551:THR:C	1:D:553:VAL:H	2.28	0.41
1:D:574:SER:HB3	1:D:613:ILE:H	1.86	0.41
1:F:49:GLY:HA2	1:F:54:TRP:CZ3	2.55	0.41
1:H:3:TRP:HB2	1:H:34:TRP:CE3	2.55	0.41
1:H:552:PRO:O	1:H:610:PRO:HB3	2.19	0.41
1:H:564:ILE:HG13	1:H:568:TRP:CZ2	2.55	0.41
1:A:426:VAL:O	1:A:426:VAL:CG1	2.68	0.41
1:C:16:THR:HG22	1:C:16:THR:O	2.19	0.41
1:C:193:PRO:HD2	1:C:194:TYR:H	1.86	0.41
1:C:301:GLY:HA2	1:C:352:ILE:O	2.21	0.41
1:C:534:CYS:HA	1:C:546:PHE:O	2.20	0.41
1:D:474:HIS:ND1	1:D:483:GLU:OE1	2.53	0.41
1:E:487:LEU:HD23	1:E:487:LEU:HA	1.89	0.41
1:E:505:LEU:HD22	1:E:572:LEU:HD12	2.02	0.41
1:F:355:ALA:HB2	1:F:375:PHE:CE2	2.55	0.41
1:H:154:TRP:HD1	1:H:466:MET:CE	2.25	0.41
1:A:55:ASP:HB3	1:A:58:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ARG:HH11	1:A:401:HIS:CE1	2.38	0.41
1:B:3:TRP:HB2	1:B:34:TRP:CZ3	2.55	0.41
1:F:145:SER:HB3	1:F:181:PHE:HA	2.01	0.41
1:F:433:LEU:HB3	1:F:448:LEU:HD21	2.03	0.41
1:A:278:ASN:OD1	1:A:332:GLU:HG2	2.21	0.41
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.85	0.41
1:C:383:TRP:CZ2	1:C:455:MET:HB2	2.55	0.41
1:D:470:PHE:CZ	1:D:484:TRP:CE3	3.09	0.41
1:E:131:MET:HE3	1:E:131:MET:HB3	1.96	0.41
1:E:421:LEU:HD11	1:E:451:LEU:HD21	2.01	0.41
1:G:53:ASN:O	1:G:54:TRP:C	2.64	0.41
1:G:515:ASP:OD1	1:G:537:ARG:NH2	2.53	0.41
1:H:125:TRP:CE3	1:H:298:HIS:HD2	2.39	0.41
1:H:172:LEU:O	1:H:176:VAL:HG23	2.20	0.41
1:H:456:TRP:HA	1:H:462:LYS:CE	2.43	0.41
1:H:564:ILE:H	1:H:564:ILE:HG12	1.58	0.41
1:B:3:TRP:O	1:B:23:LYS:NZ	2.36	0.41
1:C:456:TRP:HA	1:C:462:LYS:CE	2.45	0.41
1:E:267:HIS:NE2	1:E:309:SER:HB2	2.35	0.41
1:E:388:LEU:HD23	1:E:388:LEU:HA	1.96	0.41
1:F:87:ARG:HD3	1:F:92:GLN:OE1	2.20	0.41
1:H:101:PHE:HB2	1:H:119:THR:HG22	2.02	0.41
1:A:16:THR:HG22	1:A:16:THR:O	2.21	0.41
1:C:179:LEU:HA	1:C:500:ARG:HG3	2.03	0.41
1:C:359:THR:HG22	1:C:360:ALA:N	2.36	0.41
1:C:533:ILE:HG13	1:C:548:LEU:HD13	2.02	0.41
1:D:414:SER:C	1:D:415:GLU:HG2	2.45	0.41
1:D:455:MET:HE3	1:D:456:TRP:HZ3	1.86	0.41
1:D:526:ASN:OD1	1:D:526:ASN:O	2.39	0.41
1:E:355:ALA:HB2	1:E:375:PHE:CD2	2.56	0.41
1:E:423:HIS:HB2	1:E:476:TRP:CZ3	2.55	0.41
1:G:257:PHE:O	1:G:275:PHE:HA	2.19	0.41
1:G:421:LEU:O	1:G:463:LEU:HD23	2.20	0.41
1:G:542:ARG:HD3	1:G:542:ARG:N	2.35	0.41
1:H:149:VAL:HG12	1:H:151:LEU:HD23	2.02	0.41
1:A:149:VAL:HA	1:A:466:MET:SD	2.61	0.41
1:A:426:VAL:O	1:A:426:VAL:HG12	2.21	0.41
1:A:502:LEU:HD23	1:A:502:LEU:HA	1.90	0.41
1:E:127:ASP:CG	1:E:298:HIS:HD1	2.28	0.41
1:F:537:ARG:O	1:F:544:LEU:N	2.50	0.41
1:G:183:HIS:CD2	1:G:231:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:GLY:N	1:H:72:TYR:OH	2.54	0.41
1:A:87:ARG:HB2	1:A:92:GLN:HG2	2.02	0.41
1:A:472:GLN:CD	1:A:483:GLU:HG3	2.46	0.41
1:A:487:LEU:HA	1:A:487:LEU:HD23	1.77	0.41
1:B:3:TRP:CE2	1:B:23:LYS:HD3	2.55	0.41
1:B:150:HIS:HA	2:B:715:HOH:O	2.21	0.41
1:B:191:GLU:CD	1:B:209:THR:HA	2.46	0.41
1:B:201:GLN:C	1:B:242:ALA:HB2	2.46	0.41
1:B:342:GLU:HG3	1:B:368:THR:HG21	2.03	0.41
1:C:377:TYR:HB3	1:C:418:ILE:HG13	2.02	0.41
1:C:394:ASP:HB3	1:C:397:HIS:CD2	2.55	0.41
1:D:140:LEU:HD23	1:D:140:LEU:HA	1.91	0.41
1:E:19:ASP:OD1	1:E:19:ASP:N	2.54	0.41
1:E:148:GLU:HB3	1:E:465:PHE:HD1	1.84	0.41
1:E:255:THR:HA	1:E:258:GLU:CD	2.45	0.41
1:E:522:TRP:CZ3	1:E:533:ILE:HD12	2.56	0.41
1:E:570:GLU:O	1:E:570:GLU:HG3	2.20	0.41
1:F:150:HIS:HB2	1:F:187:LEU:HD13	2.02	0.41
1:F:330:ASN:O	1:F:334:ILE:HG13	2.20	0.41
1:F:395:PRO:CB	1:F:552:PRO:HD3	2.51	0.41
1:G:313:ARG:NH2	1:G:332:GLU:OE2	2.54	0.41
1:G:365:SER:O	1:G:365:SER:OG	2.35	0.41
1:G:419:LEU:N	1:G:461:LYS:O	2.37	0.41
1:G:420:PRO:O	1:G:421:LEU:C	2.63	0.41
1:G:570:GLU:OE2	1:G:586:ASN:HB2	2.21	0.41
1:G:575:ASP:OD2	1:G:582:SER:HB3	2.21	0.41
1:H:434:TRP:CA	1:H:448:LEU:HD11	2.49	0.41
1:A:481:GLN:NE2	2:A:702:HOH:O	2.53	0.41
1:B:332:GLU:H	1:B:332:GLU:HG3	1.43	0.41
1:B:555:ARG:HG3	1:B:555:ARG:HH11	1.86	0.41
1:C:75:GLY:O	1:C:77:LEU:HG	2.21	0.41
1:F:44:ALA:HB3	1:F:87:ARG:HB3	2.03	0.41
1:F:280:PRO:O	1:F:284:ASN:ND2	2.54	0.41
1:H:437:MET:CG	1:H:447:ASN:HB3	2.48	0.41
1:H:524:ASP:OD2	1:H:598:HIS:NE2	2.54	0.41
1:A:34:TRP:CZ3	1:A:72:TYR:HB2	2.57	0.40
1:A:107:THR:HG1	1:A:109:SER:H	1.66	0.40
1:D:6:GLU:OE1	1:D:6:GLU:N	2.42	0.40
1:D:114:LEU:HD12	1:D:114:LEU:HA	1.78	0.40
1:E:105:PRO:HA	1:E:114:LEU:H	1.85	0.40
1:E:572:LEU:HD12	1:E:615:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:LEU:HD13	1:F:361:TRP:CE3	2.56	0.40
1:H:301:GLY:HA2	1:H:352:ILE:O	2.21	0.40
1:A:176:VAL:HG13	1:A:181:PHE:HB2	2.03	0.40
1:A:571:VAL:HG21	1:A:617:GLU:HB2	2.02	0.40
1:A:571:VAL:CG2	1:A:617:GLU:HB2	2.52	0.40
1:B:19:ASP:OD2	1:B:22:ARG:CZ	2.70	0.40
1:B:30:GLU:H	1:B:30:GLU:HG2	1.44	0.40
1:B:442:TRP:HH2	1:B:610:PRO:HB2	1.86	0.40
1:D:596:SER:HA	1:D:600:ARG:O	2.21	0.40
1:F:311:LEU:HD13	1:F:361:TRP:CD2	2.56	0.40
1:G:176:VAL:HG13	1:G:181:PHE:HB2	2.03	0.40
1:A:125:TRP:HB3	1:A:127:ASP:OD1	2.21	0.40
1:A:552:PRO:O	1:A:610:PRO:HB3	2.21	0.40
1:A:576:ALA:HB3	1:A:579:TYR:CD2	2.56	0.40
1:B:192:HIS:CD2	1:B:199:GLY:HA2	2.56	0.40
1:B:456:TRP:HA	1:B:462:LYS:HE3	2.03	0.40
1:C:354:ILE:HG12	1:C:377:TYR:HB2	2.03	0.40
1:C:572:LEU:HD23	1:C:572:LEU:HA	1.96	0.40
1:D:16:THR:O	1:D:16:THR:HG22	2.21	0.40
1:A:188:PRO:HG3	1:A:235:ASP:HB3	2.03	0.40
1:B:512:LEU:HD23	1:B:537:ARG:HG2	2.04	0.40
1:D:68:LEU:HD23	1:D:68:LEU:HA	1.92	0.40
1:G:136:GLY:HA3	1:G:137:PRO:HD3	1.95	0.40
1:G:597:TRP:HB2	1:G:603:HIS:HB3	2.02	0.40
1:H:170:GLU:HA	1:H:224:TYR:HE2	1.87	0.40
1:H:523:ILE:HD11	1:H:536:LEU:HD13	2.04	0.40
1:A:601:PRO:HB2	1:A:602:PHE:CD1	2.56	0.40
1:B:191:GLU:OE1	1:B:209:THR:HA	2.22	0.40
1:B:393:ARG:HE	1:B:401:HIS:CD2	2.39	0.40
1:C:571:VAL:HG22	1:C:615:ILE:O	2.21	0.40
1:D:49:GLY:HA3	1:D:51:PHE:CE1	2.56	0.40
1:D:143:PRO:HD3	1:D:513:TRP:CE2	2.57	0.40
1:E:105:PRO:HG3	1:E:210:PHE:CE2	2.56	0.40
1:E:365:SER:HA	1:E:375:PHE:O	2.22	0.40
1:G:12:TRP:HA	1:G:284:ASN:HD21	1.86	0.40
1:G:105:PRO:HA	1:G:106:PRO:HD3	1.90	0.40
1:H:28:PRO:HA	1:H:33:THR:HG22	2.03	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	597/620 (96%)	577 (97%)	19 (3%)	1 (0%)	43	71
1	B	599/620 (97%)	580 (97%)	18 (3%)	1 (0%)	43	71
1	C	602/620 (97%)	582 (97%)	19 (3%)	1 (0%)	43	71
1	D	593/620 (96%)	571 (96%)	21 (4%)	1 (0%)	43	71
1	E	598/620 (96%)	576 (96%)	21 (4%)	1 (0%)	43	71
1	F	587/620 (95%)	558 (95%)	28 (5%)	1 (0%)	43	71
1	G	600/620 (97%)	576 (96%)	23 (4%)	1 (0%)	43	71
1	H	597/620 (96%)	582 (98%)	14 (2%)	1 (0%)	43	71
All	All	4773/4960 (96%)	4602 (96%)	163 (3%)	8 (0%)	43	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	PRO
1	B	420	PRO
1	E	420	PRO
1	F	420	PRO
1	H	420	PRO
1	D	420	PRO
1	C	420	PRO
1	G	420	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	490/528 (93%)	468 (96%)	22 (4%)	24	56
1	B	497/528 (94%)	479 (96%)	18 (4%)	31	63
1	C	496/528 (94%)	470 (95%)	26 (5%)	21	50
1	D	494/528 (94%)	468 (95%)	26 (5%)	20	50
1	E	496/528 (94%)	474 (96%)	22 (4%)	25	57
1	F	494/528 (94%)	468 (95%)	26 (5%)	20	50
1	G	494/528 (94%)	475 (96%)	19 (4%)	29	62
1	H	472/528 (89%)	445 (94%)	27 (6%)	18	48
All	All	3933/4224 (93%)	3747 (95%)	186 (5%)	23	55

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	24	LEU
1	A	29	ASP
1	A	61	LEU
1	A	83	LYS
1	A	107	THR
1	A	145	SER
1	A	178	ASP
1	A	248	LEU
1	A	270	TRP
1	A	303	ARG
1	A	394	ASP
1	A	409	LEU
1	A	419	LEU
1	A	422	SER
1	A	426	VAL
1	A	432	SER
1	A	496	GLN
1	A	538	LYS
1	A	543	LEU
1	A	556	GLU
1	A	613	ILE
1	B	13	GLU
1	B	14	SER
1	B	29	ASP
1	B	30	GLU
1	B	37	VAL

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Mol	Chain	Res	Type
1	B	111	ILE
1	B	114	LEU
1	B	117	ILE
1	B	122	ASP
1	B	153	SER
1	B	258	GLU
1	B	331	LEU
1	B	332	GLU
1	B	339	LYS
1	B	353	THR
1	B	424	ASP
1	B	451	LEU
1	B	587	PHE
1	C	2	SER
1	C	9	ILE
1	C	57	GLU
1	C	107	THR
1	C	109	SER
1	C	111	ILE
1	C	114	LEU
1	C	134	ARG
1	C	135	LYS
1	C	184	VAL
1	C	234	LEU
1	C	258	GLU
1	C	261	ASP
1	C	264	MET
1	C	274	VAL
1	C	299	VAL
1	C	314	ASP
1	C	332	GLU
1	C	422	SER
1	C	480	THR
1	C	481	GLN
1	C	528	ARG
1	C	538	LYS
1	C	551	THR
1	C	582	SER
1	C	613	ILE
1	D	14	SER
1	D	29	ASP
1	D	48	LEU

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Mol	Chain	Res	Type
1	D	114	LEU
1	D	117	ILE
1	D	145	SER
1	D	179	LEU
1	D	189	ILE
1	D	214	THR
1	D	270	TRP
1	D	274	VAL
1	D	409	LEU
1	D	414	SER
1	D	421	LEU
1	D	422	SER
1	D	451	LEU
1	D	470	PHE
1	D	480	THR
1	D	483	GLU
1	D	505	LEU
1	D	518	GLU
1	D	571	VAL
1	D	582	SER
1	D	584	MET
1	D	590	VAL
1	D	605	GLU
1	E	2	SER
1	E	14	SER
1	E	24	LEU
1	E	37	VAL
1	E	107	THR
1	E	109	SER
1	E	142	GLU
1	E	155	ARG
1	E	157	LYS
1	E	164	SER
1	E	209	THR
1	E	237	VAL
1	E	246	GLN
1	E	270	TRP
1	E	314	ASP
1	E	332	GLU
1	E	394	ASP
1	E	474	HIS
1	E	507	ARG

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Mol	Chain	Res	Type
1	E	569	ARG
1	E	613	ILE
1	E	615	ILE
1	F	4	LEU
1	F	24	LEU
1	F	29	ASP
1	F	37	VAL
1	F	122	ASP
1	F	214	THR
1	F	258	GLU
1	F	332	GLU
1	F	392	ARG
1	F	421	LEU
1	F	422	SER
1	F	425	GLU
1	F	448	LEU
1	F	451	LEU
1	F	462	LYS
1	F	463	LEU
1	F	479	ASP
1	F	524	ASP
1	F	536	LEU
1	F	543	LEU
1	F	556	GLU
1	F	562	VAL
1	F	605	GLU
1	F	613	ILE
1	F	614	LEU
1	F	616	LEU
1	G	37	VAL
1	G	53	ASN
1	G	107	THR
1	G	111	ILE
1	G	114	LEU
1	G	161	VAL
1	G	162	SER
1	G	189	ILE
1	G	249	VAL
1	G	270	TRP
1	G	331	LEU
1	G	332	GLU
1	G	394	ASP

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Mol	Chain	Res	Type
1	G	432	SER
1	G	462	LYS
1	G	482	LEU
1	G	526	ASN
1	G	607	THR
1	G	617	GLU
1	H	2	SER
1	H	5	THR
1	H	21	TYR
1	H	24	LEU
1	H	29	ASP
1	H	37	VAL
1	H	47	VAL
1	H	55	ASP
1	H	60	GLN
1	H	62	GLU
1	H	63	ARG
1	H	85	ARG
1	H	103	MET
1	H	114	LEU
1	H	202	VAL
1	H	246	GLN
1	H	254	THR
1	H	270	TRP
1	H	299	VAL
1	H	408	SER
1	H	472	GLN
1	H	480	THR
1	H	496	GLN
1	H	505	LEU
1	H	562	VAL
1	H	590	VAL
1	H	617	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	53	ASN
1	A	59	HIS
1	A	88	HIS
1	A	126	HIS

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Mol	Chain	Res	Type
1	A	177	GLN
1	A	227	GLN
1	A	402	HIS
1	A	473	HIS
1	A	474	HIS
1	A	514	HIS
1	A	530	GLN
1	B	53	ASN
1	B	88	HIS
1	B	132	GLN
1	B	370	ASN
1	B	530	GLN
1	C	88	HIS
1	C	126	HIS
1	C	397	HIS
1	C	474	HIS
1	C	477	ASN
1	C	492	HIS
1	C	530	GLN
1	D	278	ASN
1	D	347	HIS
1	D	489	GLN
1	D	530	GLN
1	E	41	HIS
1	E	246	GLN
1	E	341	ASN
1	E	385	HIS
1	E	504	HIS
1	E	526	ASN
1	E	539	HIS
1	F	60	GLN
1	F	80	HIS
1	F	341	ASN
1	F	504	HIS
1	F	514	HIS
1	G	347	HIS
1	G	454	HIS
1	G	485	HIS
1	G	492	HIS
1	G	526	ASN
1	G	530	GLN
1	H	60	GLN

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Mol	Chain	Res	Type
1	H	284	ASN
1	H	443	GLN
1	H	454	HIS
1	H	472	GLN
1	H	509	HIS
1	H	526	ASN
1	H	530	GLN

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	603/620 (97%)	-0.01	15 (2%)	58	48	19, 34, 56, 109	0
1	B	603/620 (97%)	-0.06	14 (2%)	61	51	17, 33, 54, 103	0
1	C	606/620 (97%)	-0.09	16 (2%)	57	47	18, 33, 60, 100	0
1	D	599/620 (96%)	0.02	11 (1%)	67	59	22, 36, 57, 93	0
1	E	604/620 (97%)	-0.00	12 (1%)	65	56	21, 38, 60, 95	0
1	F	593/620 (95%)	-0.04	13 (2%)	62	53	20, 35, 54, 79	0
1	G	606/620 (97%)	0.12	14 (2%)	61	51	22, 39, 64, 100	0
1	H	603/620 (97%)	0.50	36 (5%)	27	21	25, 48, 73, 88	0
All	All	4817/4960 (97%)	0.06	131 (2%)	56	46	17, 37, 63, 109	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	420	PRO	5.4
1	G	326	GLY	5.1
1	A	272	THR	4.6
1	C	266	HIS	4.4
1	H	585	GLY	4.3
1	G	325	PHE	4.2
1	F	271	GLY	4.2
1	H	266	HIS	4.1
1	G	529	ASP	4.1
1	H	529	ASP	3.9
1	C	265	ARG	3.9
1	D	420	PRO	3.7
1	E	587	PHE	3.7
1	D	272	THR	3.7
1	F	420	PRO	3.6
1	A	420	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	324	ILE	3.6
1	B	587	PHE	3.5
1	B	313	ARG	3.5
1	H	489	GLN	3.5
1	D	267	HIS	3.5
1	E	158	GLN	3.4
1	G	420	PRO	3.3
1	H	401	HIS	3.3
1	H	587	PHE	3.3
1	F	30	GLU	3.3
1	E	271	GLY	3.3
1	H	588	GLY	3.3
1	C	588	GLY	3.1
1	C	264	MET	3.1
1	H	267	HIS	3.0
1	H	619	GLU	3.0
1	F	524	ASP	3.0
1	H	271	GLY	3.0
1	F	272	THR	3.0
1	G	551	THR	3.0
1	B	266	HIS	3.0
1	H	19	ASP	3.0
1	C	262	PRO	3.0
1	A	64	TYR	3.0
1	C	420	PRO	3.0
1	H	550	PHE	3.0
1	A	325	PHE	2.9
1	H	162	SER	2.9
1	H	265	ARG	2.9
1	B	110	PRO	2.9
1	A	270	TRP	2.8
1	B	265	ARG	2.8
1	C	586	ASN	2.8
1	E	262	PRO	2.8
1	D	273	TYR	2.8
1	E	268	PRO	2.8
1	H	420	PRO	2.8
1	C	111	ILE	2.7
1	E	270	TRP	2.7
1	B	261	ASP	2.7
1	H	589	ARG	2.7
1	G	421	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	268	PRO	2.6
1	C	272	THR	2.6
1	F	619	GLU	2.6
1	G	107	THR	2.5
1	A	66	ALA	2.5
1	A	271	GLY	2.5
1	F	556	GLU	2.5
1	A	63	ARG	2.5
1	B	423	HIS	2.5
1	B	264	MET	2.4
1	E	588	GLY	2.4
1	H	108	GLY	2.4
1	F	2	SER	2.4
1	G	587	PHE	2.4
1	H	581	GLY	2.4
1	C	587	PHE	2.4
1	D	270	TRP	2.4
1	H	272	THR	2.4
1	E	269	ASP	2.4
1	H	500	ARG	2.4
1	H	400	TYR	2.4
1	D	214	THR	2.4
1	C	359	THR	2.4
1	H	167	GLU	2.3
1	G	530	GLN	2.3
1	H	109	SER	2.3
1	D	268	PRO	2.3
1	E	526	ASN	2.3
1	H	474	HIS	2.3
1	F	31	GLU	2.3
1	G	619	GLU	2.3
1	E	533	ILE	2.3
1	H	442	TRP	2.3
1	H	582	SER	2.3
1	H	268	PRO	2.3
1	A	327	GLY	2.3
1	A	526	ASN	2.3
1	F	543	LEU	2.3
1	B	107	THR	2.3
1	A	245	PRO	2.3
1	H	590	VAL	2.2
1	B	589	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	29	ASP	2.2
1	H	128	ASP	2.2
1	E	420	PRO	2.2
1	A	65	GLY	2.2
1	D	269	ASP	2.2
1	B	270	TRP	2.2
1	H	224	TYR	2.2
1	D	584	MET	2.1
1	H	23	LYS	2.1
1	C	270	TRP	2.1
1	E	470	PHE	2.1
1	H	486	LEU	2.1
1	C	314	ASP	2.1
1	C	263	ARG	2.1
1	F	329	GLU	2.1
1	F	332	GLU	2.1
1	B	488	ASP	2.1
1	D	467	GLY	2.1
1	D	508	THR	2.1
1	H	488	ASP	2.1
1	H	607	THR	2.1
1	B	111	ILE	2.1
1	G	315	TYR	2.1
1	H	396	VAL	2.0
1	C	134	ARG	2.0
1	G	271	GLY	2.0
1	A	111	ILE	2.0
1	G	9	ILE	2.0
1	H	414	SER	2.0
1	G	179	LEU	2.0
1	A	328	ARG	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.