



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:18 PM UTC

PDB ID : 4EQV / pdb_00004eqv
Title : Structure of Saccharomyces cerevisiae invertase
Authors : Sainz-Polo, M.A.; Sanz-Aparicio, J.
Deposited on : 2012-04-19
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

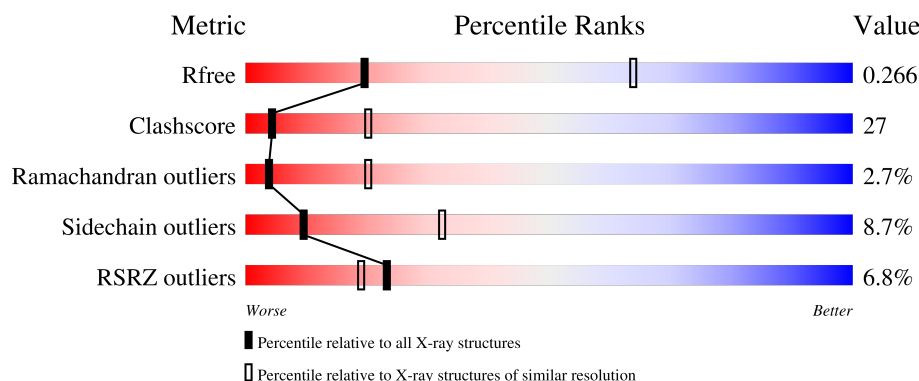
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	512	4% 70% 22% 6% ..
1	B	512	3% 69% 24% 5% ..
1	C	512	6% 68% 25% 6% ..
1	D	512	4% 69% 23% 6% ..
1	E	512	7% 64% 27% 7% ..

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Mol	Chain	Length	Quality of chain
1	F	512	7% 66% 25% 7% ..
1	G	512	12% 62% 28% 9% ..
1	H	512	12% 63% 25% 10% ..

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 33016 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 Invertase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	B	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	C	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	D	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	E	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	F	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	G	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	H	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	O	0	0
			6	6		
2	B	2	Total	O	0	0
			2	2		
2	C	4	Total	O	0	0
			4	4		
2	D	2	Total	O	0	0
			2	2		
2	E	1	Total	O	0	0
			1	1		
2	F	4	Total	O	0	0
			4	4		

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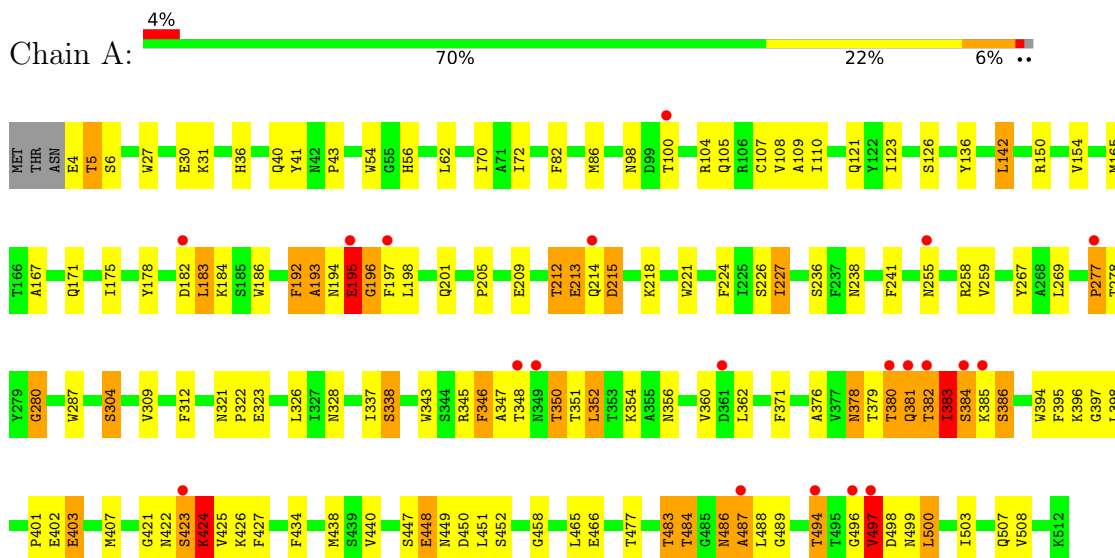
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	O	0	0
			2	2		
2	H	3	Total	O	0	0
			3	3		

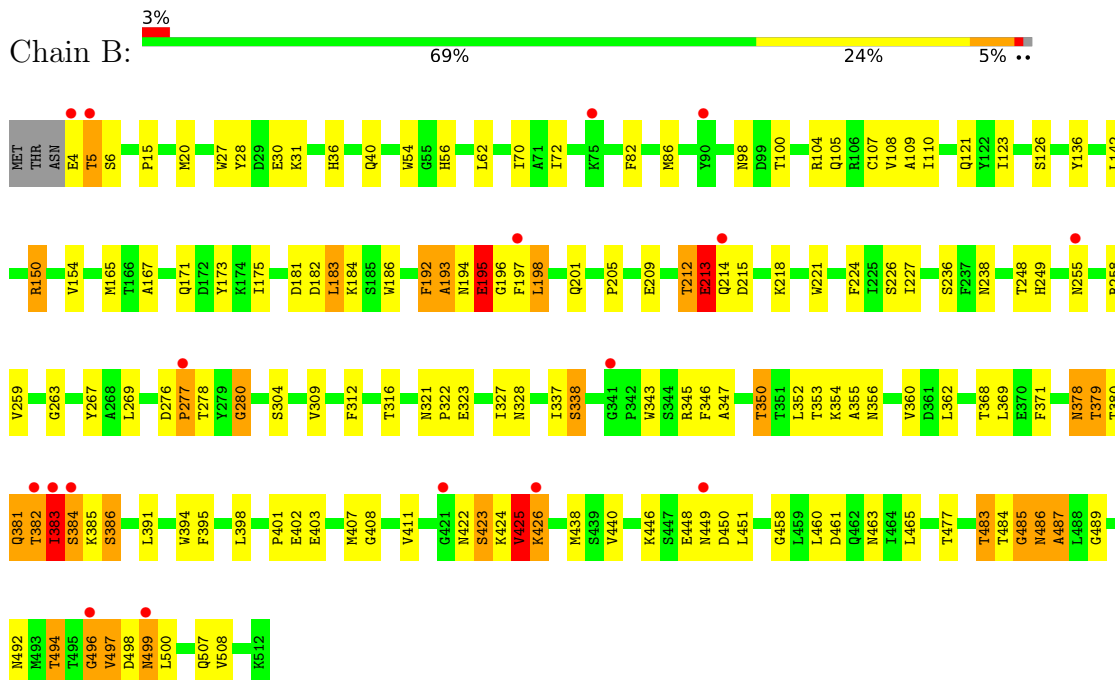
3 Residue-property plots [i](#)

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

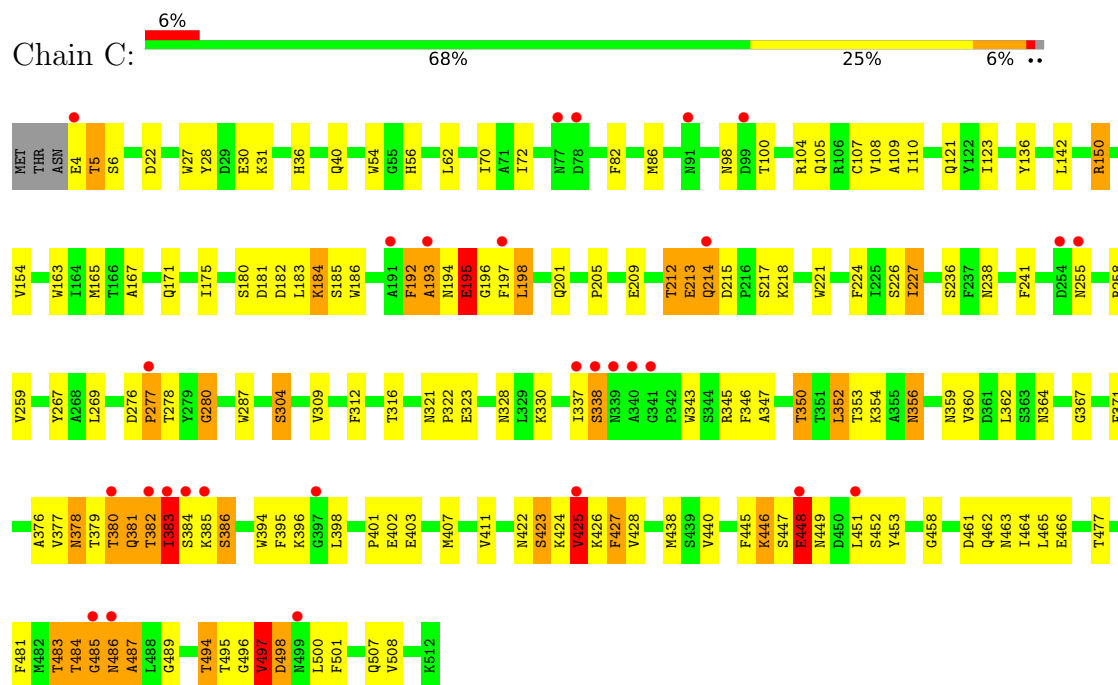
• Molecule 1: Invertase 2



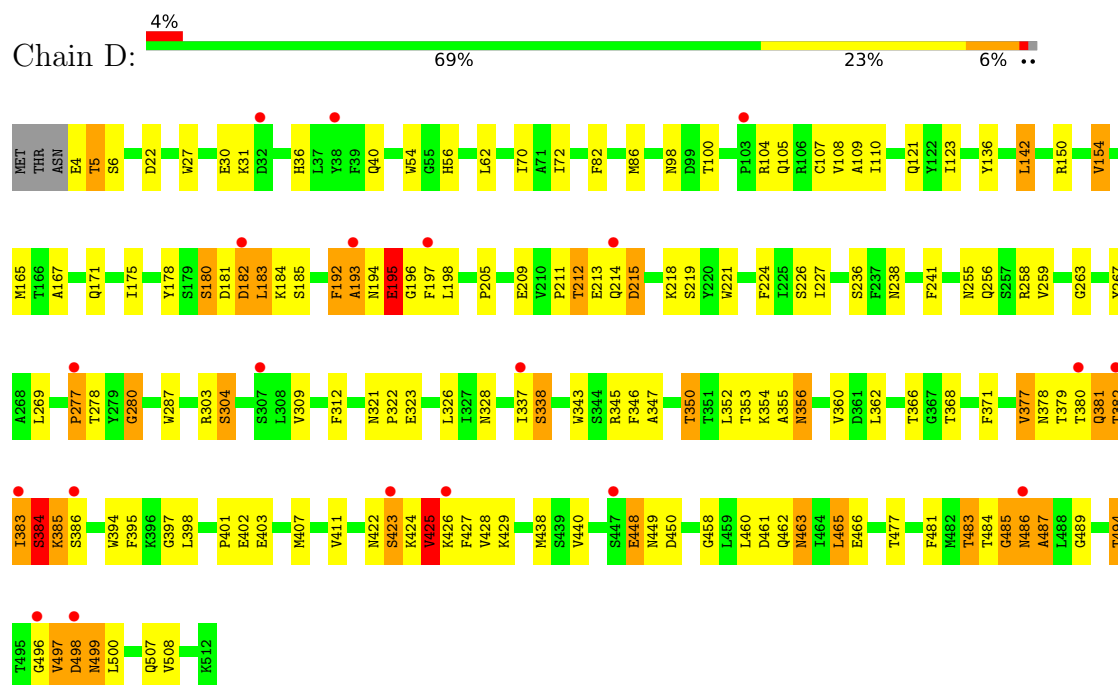
• Molecule 1: Invertase 2



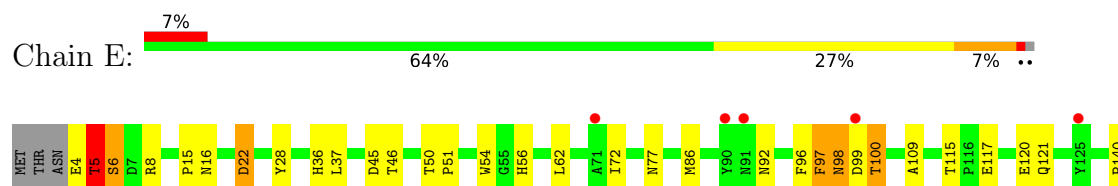
- Molecule 1: Invertase 2

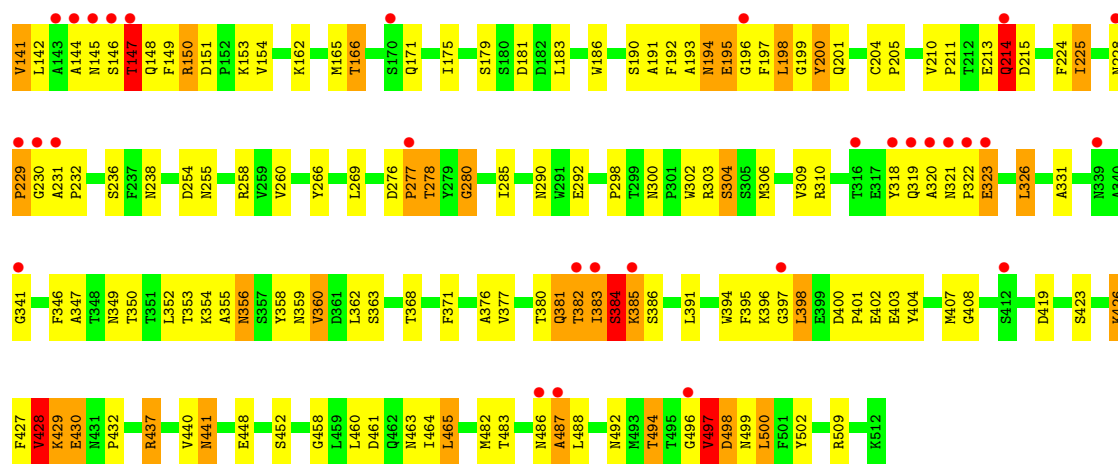


- Molecule 1: Invertase 2

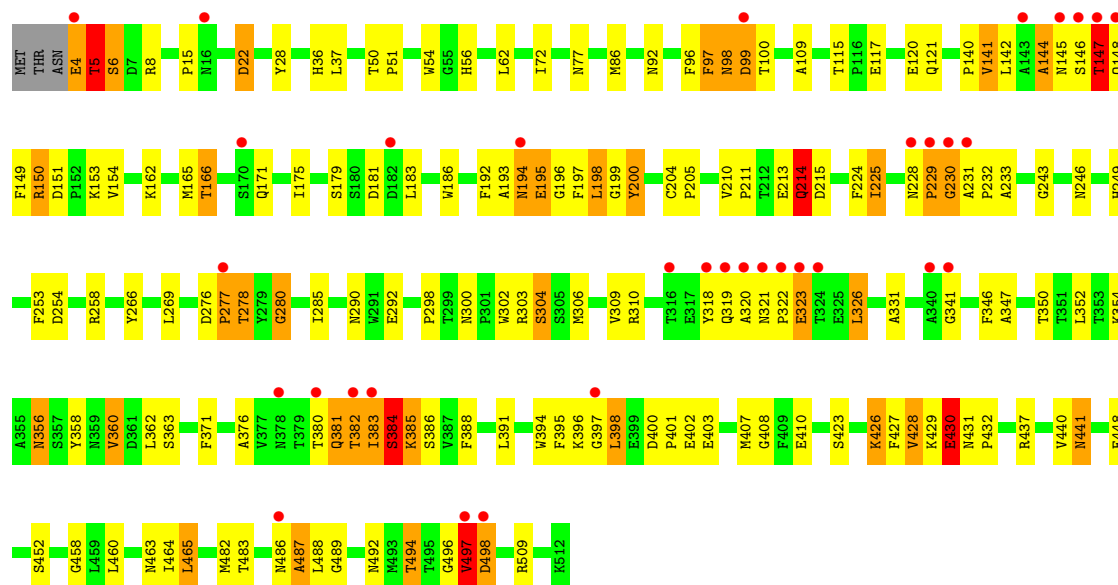


- Molecule 1: Invertase 2

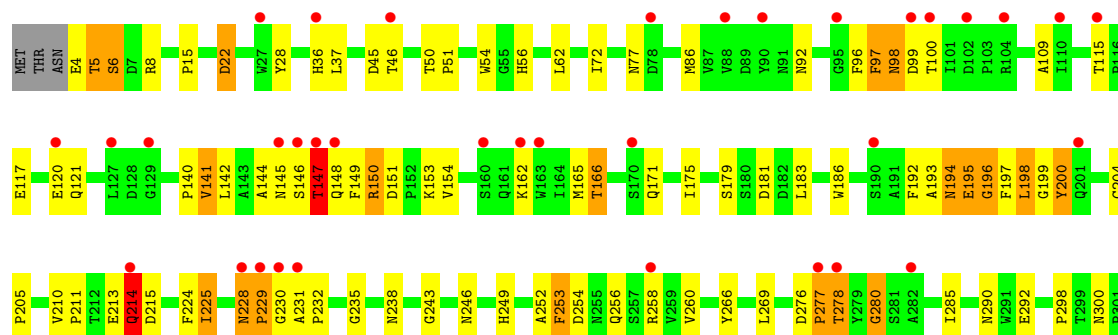


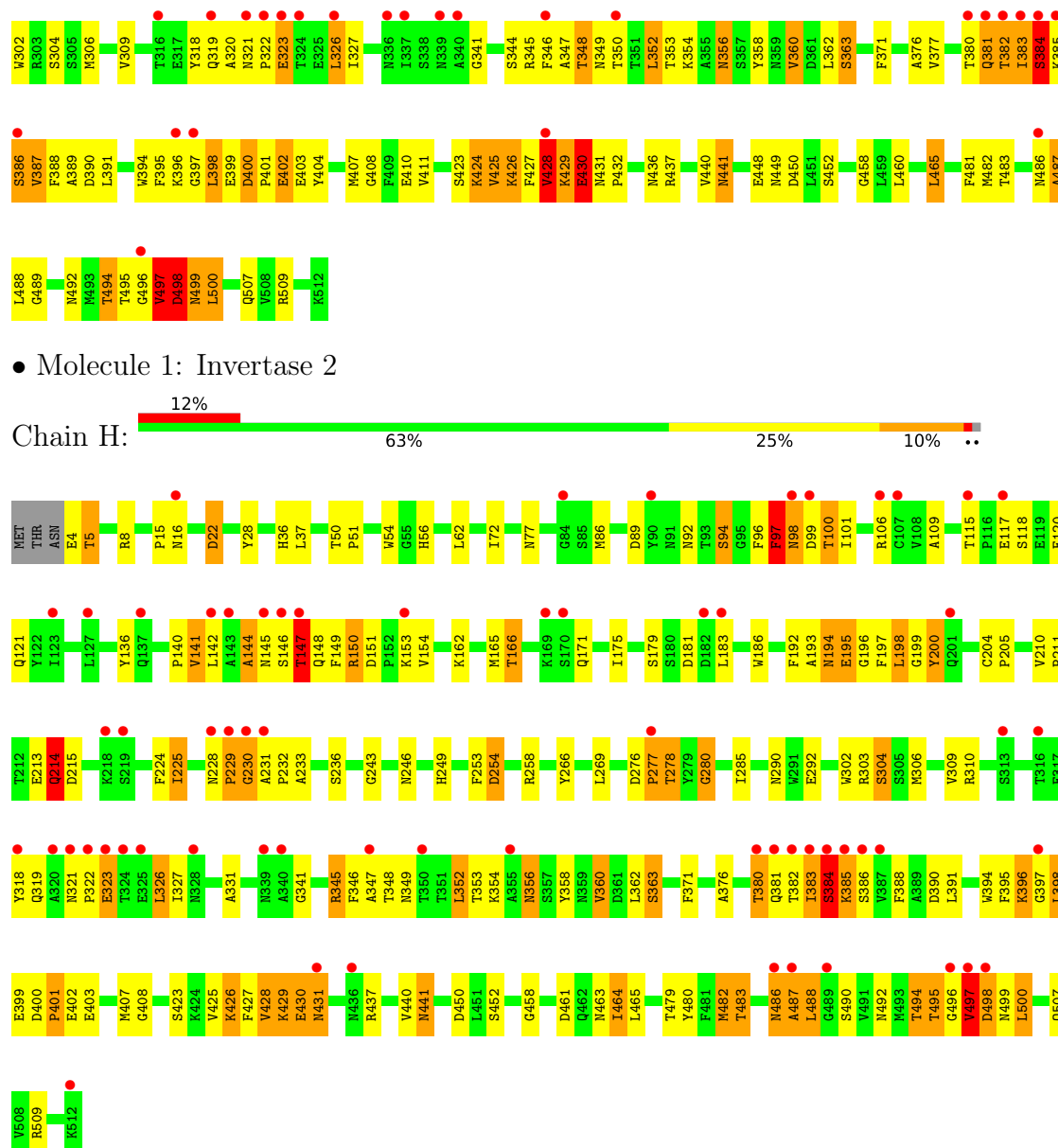


• Molecule 1: Invertase 2



• Molecule 1: Invertase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	268.66Å 268.66Å 224.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.31 – 3.40 56.31 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (56.31-3.40) 99.2 (56.31-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.221 , 0.239 0.247 , 0.266	Depositor DCC
R_{free} test set	7244 reflections (5.64%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
Reported twinning fraction	0.730 for H, K, L 0.270 for -h,-k,l	Depositor
Outliers	1 of 127516 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	33016	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1077e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.65	1/4252 (0.0%)	0.83	5/5798 (0.1%)
1	B	0.63	0/4252	0.84	7/5798 (0.1%)
1	C	0.60	0/4252	0.80	4/5798 (0.1%)
1	D	0.63	1/4252 (0.0%)	0.82	5/5798 (0.1%)
1	E	0.60	0/4252	0.85	7/5798 (0.1%)
1	F	0.61	0/4252	0.85	9/5798 (0.2%)
1	G	0.62	0/4252	0.85	14/5798 (0.2%)
1	H	0.63	2/4252 (0.0%)	0.84	8/5798 (0.1%)
All	All	0.62	4/34016 (0.0%)	0.84	59/46384 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	385	LYS	CE-NZ	-7.86	1.25	1.49
1	H	385	LYS	CD-CE	7.82	1.75	1.52
1	A	403	GLU	CD-OE1	6.09	1.36	1.25
1	D	353	THR	CB-CG2	-5.24	1.35	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	GLU	N-CA-C	-9.42	97.35	110.35
1	B	195	GLU	N-CA-C	9.12	121.30	111.36
1	A	195	GLU	N-CA-C	9.09	121.26	111.36
1	D	195	GLU	N-CA-C	7.99	120.07	111.36
1	C	195	GLU	N-CA-C	7.98	120.06	111.36
1	F	498	ASP	N-CA-C	7.58	119.54	111.28
1	C	448	GLU	N-CA-C	-7.49	101.19	110.41
1	A	346	PHE	CB-CA-C	-7.40	105.73	116.54
1	H	230	GLY	N-CA-C	-7.35	103.58	112.48
1	F	430	GLU	N-CA-C	6.97	118.96	111.36
1	F	147	THR	N-CA-C	-6.80	101.11	110.35
1	E	199	GLY	N-CA-C	-6.70	105.54	114.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	382	THR	N-CA-C	-6.65	102.25	111.30
1	E	147	THR	N-CA-C	-6.56	101.42	110.35
1	B	496	GLY	N-CA-C	-6.38	102.80	112.89
1	F	199	GLY	N-CA-C	-6.37	105.97	114.25
1	H	147	THR	N-CA-C	-6.37	101.69	110.35
1	G	254	ASP	N-CA-C	-6.32	100.93	110.28
1	G	402	GLU	N-CA-C	-6.31	100.08	113.20
1	F	382	THR	N-CA-C	-6.17	102.91	111.30
1	E	382	THR	N-CA-C	-6.16	102.92	111.30
1	G	147	THR	N-CA-C	-6.15	101.98	110.35
1	G	498	ASP	N-CA-C	6.14	117.97	111.28
1	H	199	GLY	N-CA-C	-6.08	106.34	114.25
1	G	199	GLY	N-CA-C	-6.02	106.43	114.25
1	G	430	GLU	N-CA-C	6.01	117.92	111.36
1	H	233	ALA	N-CA-C	-5.91	103.14	110.41
1	G	386	SER	N-CA-C	-5.89	100.03	109.39
1	G	99	ASP	N-CA-C	-5.77	105.41	113.37
1	E	363	SER	N-CA-C	5.76	117.56	111.28
1	D	499	ASN	N-CA-C	5.75	119.81	107.67
1	F	150	ARG	N-CA-C	5.63	115.98	108.38
1	G	150	ARG	N-CA-C	5.62	115.96	108.38
1	H	380	THR	N-CA-C	5.61	117.85	111.11
1	A	345	ARG	N-CA-C	5.60	118.20	109.52
1	G	363	SER	N-CA-C	5.59	117.37	111.28
1	H	150	ARG	N-CA-C	5.56	115.88	108.38
1	B	499	ASN	N-CA-C	5.54	119.37	107.67
1	E	150	ARG	N-CA-C	5.52	115.83	108.38
1	D	345	ARG	N-CA-C	5.51	118.05	109.52
1	B	150	ARG	N-CA-C	5.50	116.33	108.74
1	D	215	ASP	N-CA-CB	5.44	119.68	110.43
1	C	150	ARG	N-CA-C	5.43	116.23	108.74
1	F	363	SER	N-CA-C	5.42	117.19	111.28
1	B	345	ARG	N-CA-C	5.38	117.86	109.52
1	C	345	ARG	N-CA-C	5.31	117.75	109.52
1	F	5	THR	CB-CA-C	-5.29	101.68	110.68
1	F	144	ALA	N-CA-C	5.28	115.52	108.23
1	D	150	ARG	N-CA-C	5.28	116.03	108.74
1	A	215	ASP	N-CA-CB	5.27	119.38	110.43
1	B	426	LYS	N-CA-C	-5.25	105.55	111.28
1	E	99	ASP	N-CA-C	-5.18	106.21	112.54
1	H	363	SER	N-CA-C	5.13	116.88	111.28
1	G	196	GLY	N-CA-C	-5.11	106.23	112.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	228	ASN	C-N-CD	-5.08	109.43	120.60
1	H	144	ALA	N-CA-C	5.07	115.22	108.23
1	G	499	ASN	N-CA-C	5.05	116.83	108.49
1	A	487	ALA	N-CA-C	5.03	116.45	111.07
1	E	5	THR	N-CA-C	5.00	116.73	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	4124	0	3831	181	0
1	B	4124	0	3831	162	0
1	C	4124	0	3831	194	0
1	D	4124	0	3831	178	0
1	E	4124	0	3831	248	0
1	F	4124	0	3831	234	0
1	G	4124	0	3831	285	0
1	H	4124	0	3831	278	0
2	A	6	0	0	1	0
2	B	2	0	0	0	0
2	C	4	0	0	1	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	4	0	0	0	0
2	G	2	0	0	0	0
2	H	3	0	0	0	0
All	All	33016	0	30648	1705	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 27.

All (1705) 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:H:385:LYS:CE	1:H:385:LYS:CD	1.75	1.58
1:E:228:ASN:ND2	1:E:229:PRO:HB3	1.35	1.40
1:E:228:ASN:CG	1:E:229:PRO:HB3	1.47	1.38
1:F:228:ASN:ND2	1:F:229:PRO:HB3	1.35	1.37
1:H:486:ASN:HA	1:H:487:ALA:CB	1.41	1.35
1:H:97:PHE:CE2	1:H:106:ARG:HB3	1.62	1.34
1:E:192:PHE:CG	1:E:193:ALA:HB2	1.68	1.28
1:D:496:GLY:O	1:D:497:VAL:HG22	1.12	1.28
1:F:194:ASN:HA	1:F:195:GLU:CB	1.63	1.28
1:G:98:ASN:CB	1:G:100:THR:HG22	1.61	1.28
1:F:192:PHE:CG	1:F:193:ALA:HB2	1.70	1.27
1:G:256:GLN:OE1	1:G:327:ILE:HD12	1.17	1.27
1:H:194:ASN:HA	1:H:195:GLU:CB	1.62	1.27
1:G:423:SER:OG	1:G:425:VAL:HG23	1.35	1.27
1:G:192:PHE:CG	1:G:193:ALA:HB2	1.69	1.26
1:H:192:PHE:CG	1:H:193:ALA:HB2	1.70	1.25
1:E:194:ASN:HA	1:E:195:GLU:CB	1.63	1.24
1:H:228:ASN:CG	1:H:229:PRO:HG3	1.61	1.23
1:D:213:GLU:O	1:D:214:GLN:CD	1.82	1.22
1:G:194:ASN:HA	1:G:195:GLU:CB	1.63	1.22
1:E:500:LEU:HD12	1:E:500:LEU:O	1.39	1.22
1:E:486:ASN:HA	1:E:487:ALA:CB	1.65	1.21
1:F:486:ASN:HA	1:F:487:ALA:CB	1.63	1.20
1:G:486:ASN:HA	1:G:487:ALA:CB	1.66	1.20
1:G:98:ASN:HB2	1:G:100:THR:CG2	1.69	1.19
1:F:228:ASN:CG	1:F:229:PRO:HB3	1.67	1.19
1:G:385:LYS:HG3	1:G:386:SER:H	1.09	1.18
1:B:424:LYS:C	1:B:425:VAL:HG23	1.63	1.18
1:C:378:ASN:O	1:C:379:THR:HG22	1.43	1.18
1:D:378:ASN:O	1:D:379:THR:HG22	1.43	1.17
1:A:213:GLU:O	1:A:214:GLN:CD	1.90	1.15
1:H:383:ILE:N	1:H:383:ILE:HD12	1.57	1.15
1:A:398:LEU:CB	1:A:487:ALA:HB3	1.77	1.15
1:G:228:ASN:CG	1:G:229:PRO:HG3	1.71	1.15
1:D:496:GLY:O	1:D:497:VAL:CG2	1.95	1.15
1:H:97:PHE:HE2	1:H:106:ARG:CB	1.59	1.14
1:A:378:ASN:O	1:A:379:THR:HG22	1.45	1.14
1:E:98:ASN:HB2	1:E:100:THR:HG23	1.14	1.13
1:C:496:GLY:O	1:C:497:VAL:HG22	1.46	1.13
1:H:98:ASN:HB2	1:H:100:THR:HG22	1.13	1.13
1:H:97:PHE:CE2	1:H:106:ARG:CB	2.30	1.12
1:G:243:GLY:HA2	1:G:253:PHE:CE1	1.84	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:SER:HB2	1:D:185:SER:O	1.46	1.12
1:E:194:ASN:CA	1:E:195:GLU:HB3	1.79	1.12
1:F:194:ASN:CA	1:F:195:GLU:HB3	1.80	1.12
1:H:194:ASN:CA	1:H:195:GLU:HB3	1.79	1.11
1:G:243:GLY:HA2	1:G:253:PHE:CD1	1.85	1.11
1:G:194:ASN:CA	1:G:195:GLU:HB3	1.80	1.10
1:G:423:SER:OG	1:G:425:VAL:CG2	1.99	1.10
1:E:144:ALA:HB1	1:E:145:ASN:HA	1.32	1.10
1:E:398:LEU:CD1	1:E:487:ALA:O	2.00	1.10
1:H:228:ASN:OD1	1:H:229:PRO:HG3	1.52	1.10
1:A:449:ASN:ND2	1:A:450:ASP:H	1.48	1.09
1:F:144:ALA:HB1	1:F:145:ASN:HA	1.30	1.09
1:A:398:LEU:HB2	1:A:487:ALA:HB3	1.11	1.09
1:B:496:GLY:O	1:B:497:VAL:HG22	1.50	1.09
1:D:213:GLU:C	1:D:214:GLN:OE1	1.95	1.09
1:F:5:THR:O	1:F:6:SER:HB2	1.47	1.09
1:F:398:LEU:H	1:F:398:LEU:HD13	1.12	1.09
1:B:449:ASN:ND2	1:B:450:ASP:H	1.50	1.08
1:H:228:ASN:ND2	1:H:229:PRO:HB3	1.68	1.08
1:C:192:PHE:CE2	1:C:195:GLU:HG2	1.89	1.08
1:G:486:ASN:HA	1:G:487:ALA:HB2	1.34	1.07
1:C:352:LEU:H	1:C:352:LEU:CD1	1.67	1.07
1:C:352:LEU:HD12	1:C:352:LEU:N	1.66	1.07
1:E:398:LEU:HD12	1:E:487:ALA:O	1.55	1.07
1:H:486:ASN:CA	1:H:487:ALA:CB	2.30	1.07
1:H:383:ILE:HD12	1:H:383:ILE:H	1.07	1.07
1:H:228:ASN:ND2	1:H:229:PRO:HG3	1.71	1.06
1:H:486:ASN:HA	1:H:487:ALA:HB2	1.37	1.06
1:D:379:THR:HG22	1:D:450:ASP:O	1.56	1.05
1:F:486:ASN:HA	1:F:487:ALA:HB2	1.29	1.05
1:A:423:SER:O	1:A:424:LYS:HB2	1.52	1.05
1:C:362:LEU:HA	1:E:356:ASN:HB3	1.34	1.05
1:E:486:ASN:HA	1:E:487:ALA:HB2	1.33	1.05
1:G:228:ASN:ND2	1:G:229:PRO:HG3	1.72	1.05
1:H:144:ALA:HB1	1:H:145:ASN:HA	1.33	1.05
1:A:213:GLU:C	1:A:214:GLN:OE1	1.99	1.05
1:E:398:LEU:CD1	1:E:398:LEU:H	1.70	1.05
1:B:378:ASN:O	1:B:379:THR:HG22	1.54	1.04
1:E:398:LEU:HD12	1:E:398:LEU:N	1.72	1.04
1:H:144:ALA:HB1	1:H:145:ASN:CA	1.87	1.04
1:D:379:THR:CG2	1:D:450:ASP:O	2.06	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:ALA:HB1	1:F:145:ASN:CA	1.89	1.03
1:F:398:LEU:HD13	1:F:398:LEU:N	1.69	1.03
1:G:256:GLN:OE1	1:G:327:ILE:CD1	2.06	1.03
1:A:496:GLY:O	1:A:497:VAL:HG22	1.59	1.03
1:G:385:LYS:HG3	1:G:386:SER:N	1.72	1.03
1:E:144:ALA:HB1	1:E:145:ASN:CA	1.88	1.02
1:E:228:ASN:CG	1:E:229:PRO:CB	2.31	1.02
1:G:228:ASN:CG	1:G:229:PRO:CG	2.32	1.02
1:H:97:PHE:CD2	1:H:106:ARG:HG2	1.94	1.02
1:B:424:LYS:O	1:B:425:VAL:HG23	1.58	1.02
1:D:403:GLU:OE2	1:D:424:LYS:HG3	1.58	1.02
1:A:422:ASN:HA	1:A:423:SER:HB2	1.40	1.02
1:E:385:LYS:HG3	1:E:386:SER:N	1.74	1.02
1:A:212:THR:HG22	1:A:215:ASP:O	1.60	1.01
1:G:144:ALA:HB1	1:G:145:ASN:CA	1.91	1.01
1:F:147:THR:HB	1:F:171:GLN:NE2	1.75	1.01
1:H:147:THR:HB	1:H:171:GLN:NE2	1.75	1.01
1:H:228:ASN:CG	1:H:229:PRO:CG	2.32	1.01
1:G:192:PHE:CD2	1:G:193:ALA:HB2	1.96	1.01
1:E:419:ASP:OD2	1:E:437:ARG:NH1	1.93	1.01
1:G:228:ASN:ND2	1:G:229:PRO:HB3	1.74	1.01
1:A:403:GLU:OE2	1:A:424:LYS:CG	2.09	1.00
1:B:212:THR:HG23	1:B:213:GLU:O	1.57	1.00
1:H:486:ASN:HA	1:H:487:ALA:HB3	1.02	1.00
1:A:500:LEU:HD12	1:A:500:LEU:O	1.59	1.00
1:E:192:PHE:CD2	1:E:193:ALA:HB2	1.96	1.00
1:G:228:ASN:OD1	1:G:229:PRO:HG3	1.62	1.00
1:E:147:THR:HB	1:E:171:GLN:NE2	1.76	1.00
1:H:192:PHE:CD2	1:H:193:ALA:HB2	1.98	0.99
1:G:98:ASN:HD22	1:G:98:ASN:N	1.58	0.99
1:H:486:ASN:CA	1:H:487:ALA:HB3	1.92	0.99
1:F:147:THR:HB	1:F:171:GLN:HE21	1.28	0.98
1:F:192:PHE:CD2	1:F:193:ALA:HB2	1.98	0.98
1:A:362:LEU:HA	1:F:356:ASN:HB3	1.42	0.98
1:A:352:LEU:CD1	1:A:503:ILE:HG12	1.94	0.98
1:C:352:LEU:H	1:C:352:LEU:HD12	0.83	0.97
1:C:422:ASN:HA	1:C:423:SER:HB2	1.46	0.97
1:A:496:GLY:O	1:A:497:VAL:HG13	1.64	0.97
1:E:228:ASN:OD1	1:E:229:PRO:HG3	1.63	0.97
1:F:385:LYS:HG3	1:F:386:SER:N	1.78	0.97
1:E:98:ASN:HB2	1:E:100:THR:CG2	1.94	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:THR:HB	1:H:171:GLN:HE21	1.30	0.96
1:G:98:ASN:HD22	1:G:98:ASN:H	1.03	0.96
1:G:144:ALA:HB1	1:G:145:ASN:C	1.90	0.96
1:A:212:THR:HG23	1:A:213:GLU:O	1.66	0.96
1:G:147:THR:HB	1:G:171:GLN:NE2	1.81	0.96
1:B:212:THR:CG2	1:B:213:GLU:O	2.14	0.96
1:D:182:ASP:OD2	1:D:184:LYS:HG3	1.64	0.96
1:G:194:ASN:HA	1:G:195:GLU:HB3	0.96	0.96
1:G:232:PRO:HG2	1:H:441:ASN:HB2	1.47	0.95
1:E:428:VAL:O	1:F:437:ARG:NH2	1.99	0.95
1:B:379:THR:CG2	1:B:380:THR:N	2.28	0.95
1:E:194:ASN:ND2	1:E:196:GLY:H	1.64	0.95
1:H:228:ASN:ND2	1:H:229:PRO:CB	2.29	0.95
1:E:147:THR:HB	1:E:171:GLN:HE21	1.31	0.95
1:G:144:ALA:HB1	1:G:145:ASN:HA	1.45	0.95
1:H:145:ASN:N	1:H:146:SER:HA	1.81	0.95
1:H:194:ASN:ND2	1:H:196:GLY:H	1.65	0.95
1:G:194:ASN:ND2	1:G:196:GLY:H	1.65	0.95
1:F:228:ASN:ND2	1:F:229:PRO:CB	2.29	0.94
1:G:383:ILE:O	1:G:384:SER:HB2	1.65	0.94
1:G:228:ASN:ND2	1:G:229:PRO:CB	2.29	0.94
1:H:194:ASN:HA	1:H:195:GLU:HB3	0.94	0.94
1:B:424:LYS:C	1:B:425:VAL:CG2	2.38	0.94
1:F:145:ASN:N	1:F:146:SER:HA	1.80	0.94
1:F:398:LEU:HD13	1:F:487:ALA:O	1.67	0.94
1:E:486:ASN:HA	1:E:487:ALA:HB3	1.50	0.93
1:F:486:ASN:HA	1:F:487:ALA:HB3	1.50	0.93
1:H:98:ASN:CB	1:H:100:THR:HG22	1.98	0.93
1:A:496:GLY:C	1:A:497:VAL:HG13	1.94	0.93
1:H:97:PHE:HD2	1:H:106:ARG:HG2	1.29	0.93
1:F:398:LEU:N	1:F:398:LEU:CD1	2.32	0.93
1:E:228:ASN:ND2	1:E:229:PRO:CB	2.29	0.93
1:A:422:ASN:HA	1:A:423:SER:CB	1.99	0.93
1:C:448:GLU:OE1	1:C:448:GLU:HA	1.67	0.93
1:F:194:ASN:ND2	1:F:196:GLY:H	1.65	0.92
1:F:194:ASN:HA	1:F:195:GLU:HB3	0.96	0.92
1:E:145:ASN:N	1:E:146:SER:HA	1.82	0.92
1:G:228:ASN:ND2	1:G:229:PRO:CG	2.32	0.92
1:E:326:LEU:HD12	1:E:326:LEU:H	1.34	0.92
1:A:192:PHE:HD2	1:A:192:PHE:O	1.53	0.92
1:D:385:LYS:O	1:D:386:SER:HB3	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:437:ARG:NH2	1:H:428:VAL:O	2.03	0.91
1:G:385:LYS:CG	1:G:386:SER:N	2.30	0.91
1:H:228:ASN:ND2	1:H:229:PRO:CG	2.32	0.91
1:F:228:ASN:CG	1:F:229:PRO:CB	2.43	0.91
1:F:400:ASP:OD1	1:F:401:PRO:O	1.89	0.91
1:E:194:ASN:HA	1:E:195:GLU:HB3	0.95	0.90
1:E:437:ARG:NH2	1:F:428:VAL:O	2.04	0.90
1:A:379:THR:CG2	1:A:450:ASP:O	2.20	0.90
1:A:449:ASN:HD22	1:A:450:ASP:H	1.15	0.90
1:G:486:ASN:HA	1:G:487:ALA:HB3	1.50	0.90
1:E:98:ASN:CB	1:E:100:THR:HG23	2.02	0.89
1:G:437:ARG:NH1	1:H:431:ASN:O	2.04	0.89
1:H:352:LEU:HB3	1:H:495:THR:HG21	1.55	0.89
1:F:496:GLY:O	1:F:497:VAL:HG12	1.72	0.89
1:F:326:LEU:HD12	1:F:326:LEU:H	1.35	0.89
1:H:97:PHE:CD2	1:H:106:ARG:CG	2.55	0.89
1:C:423:SER:O	1:C:425:VAL:HG23	1.73	0.89
1:B:449:ASN:HD22	1:B:450:ASP:H	1.15	0.89
1:F:394:TRP:HE1	1:F:494:THR:HB	1.38	0.89
1:H:326:LEU:H	1:H:326:LEU:HD12	1.36	0.89
1:E:192:PHE:CD1	1:E:193:ALA:HB2	2.09	0.88
1:H:383:ILE:N	1:H:383:ILE:CD1	2.33	0.88
1:F:98:ASN:HB2	1:F:100:THR:HG22	1.54	0.88
1:F:192:PHE:CD1	1:F:193:ALA:HB2	2.07	0.88
1:C:192:PHE:CZ	1:C:195:GLU:CG	2.57	0.88
1:B:446:LYS:NZ	1:B:448:GLU:OE2	2.04	0.88
1:C:192:PHE:CZ	1:C:195:GLU:HG2	2.09	0.88
1:H:323:GLU:OE2	1:H:323:GLU:HA	1.74	0.88
1:H:192:PHE:CD1	1:H:193:ALA:HB2	2.08	0.88
1:C:378:ASN:C	1:C:378:ASN:HD22	1.81	0.87
1:G:192:PHE:CD1	1:G:193:ALA:HB2	2.09	0.87
1:A:213:GLU:HB3	1:A:214:GLN:OE1	1.74	0.87
1:C:182:ASP:O	1:C:183:LEU:HB2	1.74	0.87
1:F:397:GLY:O	1:F:487:ALA:O	1.92	0.87
1:A:403:GLU:OE2	1:A:424:LYS:CB	2.22	0.87
1:H:198:LEU:C	1:H:198:LEU:HD12	1.99	0.87
1:G:395:PHE:HE2	1:G:407:MET:HE2	1.36	0.87
1:G:5:THR:O	1:G:6:SER:HB2	1.75	0.86
1:B:422:ASN:HA	1:B:423:SER:HB2	1.56	0.86
1:D:403:GLU:OE2	1:D:424:LYS:CG	2.24	0.86
1:E:323:GLU:OE2	1:E:323:GLU:HA	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:GLU:OE2	1:F:323:GLU:HA	1.74	0.86
1:G:326:LEU:HD12	1:G:326:LEU:H	1.37	0.86
1:B:382:THR:C	1:B:383:ILE:HG12	2.00	0.86
1:E:198:LEU:C	1:E:198:LEU:HD12	2.00	0.86
1:H:346:PHE:CE1	1:H:360:VAL:HG23	2.10	0.86
1:F:198:LEU:C	1:F:198:LEU:HD12	2.01	0.86
1:G:147:THR:HB	1:G:171:GLN:HE21	1.36	0.86
1:G:323:GLU:HA	1:G:323:GLU:OE2	1.75	0.86
1:E:194:ASN:HD22	1:E:196:GLY:H	1.24	0.86
1:H:92:ASN:OD1	1:H:96:PHE:O	1.93	0.86
1:D:212:THR:HG22	1:D:215:ASP:O	1.76	0.86
1:H:427:PHE:O	1:H:427:PHE:CD2	2.29	0.85
1:E:398:LEU:HD12	1:E:398:LEU:H	1.28	0.85
1:A:379:THR:CG2	1:A:380:THR:N	2.40	0.85
1:C:380:THR:O	1:C:380:THR:HG22	1.75	0.85
1:B:192:PHE:CD2	1:B:192:PHE:O	2.30	0.85
1:G:441:ASN:HB2	1:H:232:PRO:HG2	1.59	0.85
1:A:379:THR:HG23	1:A:380:THR:N	1.91	0.84
1:E:398:LEU:CD1	1:E:398:LEU:N	2.35	0.84
1:B:379:THR:HG22	1:B:380:THR:H	1.41	0.84
1:E:394:TRP:HE1	1:E:494:THR:HB	1.42	0.84
1:E:427:PHE:O	1:E:427:PHE:CD2	2.30	0.84
1:H:144:ALA:HB1	1:H:145:ASN:C	2.01	0.84
1:G:198:LEU:C	1:G:198:LEU:HD12	2.01	0.84
1:G:396:LYS:HG2	1:G:404:TYR:HB3	1.60	0.84
1:H:385:LYS:CD	1:H:385:LYS:NZ	2.41	0.84
1:A:192:PHE:O	1:A:192:PHE:CD2	2.31	0.84
1:A:500:LEU:HD12	1:A:500:LEU:C	1.99	0.84
1:E:497:VAL:HG12	1:E:497:VAL:O	1.78	0.84
1:A:378:ASN:C	1:A:378:ASN:HD22	1.84	0.84
1:B:238:ASN:HD21	1:B:269:LEU:H	1.25	0.84
1:D:422:ASN:HA	1:D:423:SER:HB2	1.59	0.84
1:D:195:GLU:OE2	1:D:195:GLU:HA	1.76	0.83
1:F:427:PHE:O	1:F:427:PHE:CD2	2.31	0.83
1:F:194:ASN:HD22	1:F:196:GLY:H	1.25	0.83
1:D:238:ASN:HD21	1:D:269:LEU:H	1.26	0.83
1:G:243:GLY:CA	1:G:253:PHE:CE1	2.60	0.83
1:E:144:ALA:HB1	1:E:145:ASN:C	2.03	0.83
1:G:394:TRP:HE1	1:G:494:THR:HB	1.41	0.83
1:C:238:ASN:HD21	1:C:269:LEU:H	1.26	0.82
1:E:194:ASN:CA	1:E:195:GLU:CB	2.48	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:THR:HG22	1:B:380:THR:N	1.93	0.82
1:H:353:THR:HB	1:H:498:ASP:OD1	1.79	0.82
1:G:318:TYR:HD2	1:G:319:GLN:O	1.63	0.82
1:G:395:PHE:CE2	1:G:407:MET:HE2	2.15	0.82
1:F:398:LEU:HD11	1:F:489:GLY:HA3	1.62	0.82
1:H:194:ASN:HD22	1:H:196:GLY:H	1.25	0.81
1:C:496:GLY:O	1:C:497:VAL:CG2	2.28	0.81
1:D:213:GLU:O	1:D:214:GLN:OE1	1.91	0.81
1:F:326:LEU:HD12	1:F:326:LEU:N	1.96	0.81
1:A:496:GLY:O	1:A:497:VAL:CG2	2.28	0.81
1:D:496:GLY:C	1:D:497:VAL:HG22	2.03	0.81
1:F:318:TYR:HD2	1:F:319:GLN:O	1.63	0.81
1:A:238:ASN:HD21	1:A:269:LEU:H	1.26	0.81
1:B:356:ASN:HB3	1:G:362:LEU:HA	1.62	0.81
1:E:318:TYR:HD2	1:E:319:GLN:O	1.63	0.81
1:C:323:GLU:HG2	1:D:171:GLN:HE21	1.46	0.81
1:E:326:LEU:HD12	1:E:326:LEU:N	1.95	0.81
1:H:318:TYR:HD2	1:H:319:GLN:O	1.62	0.81
1:G:381:GLN:O	1:G:382:THR:C	2.23	0.81
1:H:96:PHE:C	1:H:97:PHE:HD1	1.87	0.81
1:H:97:PHE:HE2	1:H:106:ARG:CA	1.93	0.81
1:D:379:THR:HG23	1:D:380:THR:N	1.95	0.81
1:E:347:ALA:HB1	1:E:350:THR:HG21	1.63	0.81
1:H:383:ILE:H	1:H:383:ILE:CD1	1.78	0.80
1:F:4:GLU:N	1:F:4:GLU:CD	2.37	0.80
1:E:5:THR:O	1:E:300:ASN:O	2.00	0.80
1:A:192:PHE:CZ	1:A:195:GLU:HG2	2.16	0.80
1:H:231:ALA:H	1:H:232:PRO:HD2	1.46	0.80
1:A:403:GLU:OE2	1:A:424:LYS:HG3	1.80	0.80
1:F:496:GLY:O	1:F:497:VAL:CB	2.30	0.80
1:C:213:GLU:O	1:C:214:GLN:CG	2.30	0.80
1:G:346:PHE:CE1	1:G:360:VAL:HG23	2.17	0.80
1:B:497:VAL:HG23	1:B:497:VAL:O	1.82	0.80
1:D:195:GLU:OE2	1:D:195:GLU:CA	2.30	0.80
1:F:228:ASN:OD1	1:F:229:PRO:CG	2.30	0.80
1:G:92:ASN:OD1	1:G:96:PHE:O	1.98	0.80
1:H:385:LYS:CE	1:H:385:LYS:CG	2.60	0.79
1:D:497:VAL:HG23	1:D:497:VAL:O	1.82	0.79
1:F:347:ALA:HB1	1:F:350:THR:HG21	1.62	0.79
1:F:427:PHE:O	1:F:428:VAL:HG23	1.82	0.79
1:H:144:ALA:CB	1:H:145:ASN:HA	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:THR:CG2	1:C:380:THR:N	2.46	0.79
1:H:98:ASN:ND2	1:H:98:ASN:N	2.31	0.79
1:F:144:ALA:HB1	1:F:145:ASN:C	2.08	0.79
1:A:379:THR:HG22	1:A:450:ASP:O	1.81	0.79
1:B:192:PHE:O	1:B:192:PHE:HD2	1.65	0.79
1:B:362:LEU:HA	1:G:356:ASN:HB3	1.65	0.79
1:B:449:ASN:ND2	1:B:450:ASP:N	2.31	0.79
1:C:496:GLY:C	1:C:497:VAL:HG13	2.05	0.79
1:G:194:ASN:HD22	1:G:196:GLY:H	1.26	0.79
1:E:228:ASN:OD1	1:E:229:PRO:CG	2.30	0.79
1:E:96:PHE:O	1:E:97:PHE:CD1	2.36	0.79
1:G:145:ASN:N	1:G:146:SER:HA	1.97	0.79
1:G:496:GLY:C	1:G:497:VAL:HG13	2.07	0.79
1:C:445:PHE:CE1	1:C:446:LYS:HD3	2.18	0.79
1:D:394:TRP:HE1	1:D:494:THR:HB	1.48	0.79
1:E:353:THR:HA	1:E:498:ASP:O	1.83	0.79
1:E:497:VAL:O	1:E:497:VAL:CG1	2.30	0.79
1:F:290:ASN:OD1	1:F:292:GLU:HG2	1.83	0.79
1:C:192:PHE:C	1:C:192:PHE:CD2	2.60	0.78
1:H:147:THR:CB	1:H:171:GLN:NE2	2.47	0.78
1:C:180:SER:HB2	1:C:185:SER:O	1.83	0.78
1:F:228:ASN:OD1	1:F:229:PRO:HD3	1.83	0.78
1:H:326:LEU:HD12	1:H:326:LEU:N	1.97	0.78
1:E:98:ASN:CB	1:E:100:THR:CG2	2.61	0.78
1:E:427:PHE:O	1:E:427:PHE:CG	2.34	0.78
1:H:98:ASN:N	1:H:98:ASN:HD22	1.79	0.78
1:B:496:GLY:O	1:B:497:VAL:CG2	2.30	0.78
1:C:192:PHE:HD2	1:C:192:PHE:O	1.67	0.78
1:G:228:ASN:CG	1:G:229:PRO:HB3	2.09	0.78
1:G:326:LEU:HD12	1:G:326:LEU:N	1.97	0.78
1:B:212:THR:HG22	1:B:215:ASP:O	1.84	0.78
1:D:385:LYS:HG3	1:D:386:SER:H	1.48	0.78
1:E:5:THR:O	1:E:6:SER:CB	2.30	0.78
1:F:228:ASN:OD1	1:F:229:PRO:CD	2.32	0.78
1:G:5:THR:HG22	1:G:6:SER:O	1.83	0.78
1:E:92:ASN:OD1	1:E:96:PHE:O	2.02	0.78
1:E:192:PHE:CD2	1:E:193:ALA:CB	2.67	0.78
1:A:449:ASN:ND2	1:A:450:ASP:N	2.30	0.78
1:F:144:ALA:CB	1:F:145:ASN:HA	2.11	0.78
1:A:394:TRP:HE1	1:A:494:THR:HB	1.47	0.78
1:C:394:TRP:HE1	1:C:494:THR:HB	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLN:HE21	1:B:323:GLU:HG2	1.49	0.77
1:F:147:THR:CB	1:F:171:GLN:NE2	2.47	0.77
1:F:496:GLY:O	1:F:497:VAL:CG1	2.31	0.77
1:A:403:GLU:OE2	1:A:483:THR:HB	1.84	0.77
1:E:290:ASN:OD1	1:E:292:GLU:HG2	1.83	0.77
1:H:97:PHE:HD2	1:H:106:ARG:CG	1.94	0.77
1:A:192:PHE:CD2	1:A:192:PHE:C	2.62	0.77
1:A:496:GLY:O	1:A:497:VAL:CG1	2.32	0.77
1:C:497:VAL:CG2	1:C:497:VAL:O	2.31	0.77
1:E:144:ALA:CB	1:E:145:ASN:HA	2.12	0.77
1:G:232:PRO:CG	1:H:441:ASN:HB2	2.14	0.77
1:D:379:THR:HG21	1:D:450:ASP:O	1.84	0.77
1:G:192:PHE:CD2	1:G:193:ALA:CB	2.67	0.77
1:G:427:PHE:O	1:G:428:VAL:HG23	1.84	0.77
1:C:485:GLY:O	1:C:486:ASN:HB2	1.85	0.77
1:H:290:ASN:OD1	1:H:292:GLU:HG2	1.84	0.77
1:B:394:TRP:HE1	1:B:494:THR:HB	1.48	0.77
1:E:147:THR:CB	1:E:171:GLN:NE2	2.47	0.77
1:E:298:PRO:HD3	1:E:427:PHE:CD2	2.19	0.77
1:F:395:PHE:HE2	1:F:407:MET:HE2	1.49	0.76
1:G:290:ASN:OD1	1:G:292:GLU:HG2	1.85	0.76
1:H:427:PHE:O	1:H:428:VAL:HG23	1.84	0.76
1:F:347:ALA:CB	1:F:350:THR:HG21	2.15	0.76
1:G:5:THR:O	1:G:300:ASN:O	2.04	0.76
1:C:379:THR:HG23	1:C:380:THR:N	1.98	0.76
1:G:231:ALA:H	1:G:232:PRO:HD2	1.49	0.76
1:B:403:GLU:OE2	1:B:483:THR:HB	1.85	0.76
1:D:356:ASN:HB3	1:H:362:LEU:HA	1.67	0.76
1:D:485:GLY:O	1:D:486:ASN:HB2	1.84	0.76
1:E:500:LEU:HD12	1:E:500:LEU:C	2.06	0.76
1:G:428:VAL:HG12	1:G:429:LYS:N	1.99	0.76
1:D:378:ASN:O	1:D:379:THR:CG2	2.31	0.76
1:D:379:THR:CG2	1:D:380:THR:N	2.48	0.76
1:G:147:THR:HA	1:G:171:GLN:HE22	1.51	0.76
1:C:403:GLU:OE2	1:C:483:THR:HB	1.86	0.76
1:C:214:GLN:HG2	1:C:215:ASP:H	1.51	0.75
1:B:277:PRO:HB3	1:B:280:GLY:HA2	1.67	0.75
1:H:192:PHE:CD2	1:H:193:ALA:CB	2.69	0.75
1:G:228:ASN:OD1	1:G:229:PRO:CG	2.31	0.75
1:G:388:PHE:CE2	1:G:390:ASP:HB3	2.21	0.75
1:A:378:ASN:O	1:A:379:THR:CG2	2.31	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ASN:O	1:B:379:THR:CG2	2.34	0.75
1:C:403:GLU:OE2	1:C:424:LYS:HG3	1.86	0.75
1:H:231:ALA:HB3	1:H:232:PRO:HD3	1.68	0.75
1:C:192:PHE:CZ	1:C:195:GLU:HG3	2.21	0.75
1:G:121:GLN:HG3	1:G:149:PHE:HE2	1.52	0.75
1:H:488:LEU:HD23	1:H:488:LEU:N	2.01	0.75
1:C:352:LEU:CD1	1:C:501:PHE:O	2.35	0.75
1:G:228:ASN:CG	1:G:229:PRO:CB	2.57	0.75
1:G:496:GLY:O	1:G:497:VAL:HG22	1.85	0.75
1:A:378:ASN:C	1:A:378:ASN:ND2	2.42	0.75
1:B:424:LYS:O	1:B:425:VAL:CG2	2.32	0.75
1:E:347:ALA:CB	1:E:350:THR:HG21	2.16	0.74
1:H:96:PHE:C	1:H:97:PHE:CD1	2.64	0.74
1:F:460:LEU:HG	1:F:465:LEU:HD12	1.68	0.74
1:G:383:ILE:O	1:G:384:SER:CB	2.35	0.74
1:D:277:PRO:HB3	1:D:280:GLY:HA2	1.67	0.74
1:D:403:GLU:OE2	1:D:483:THR:HB	1.87	0.74
1:E:419:ASP:CG	1:E:437:ARG:HH11	1.93	0.74
1:G:231:ALA:HB3	1:G:232:PRO:HD3	1.70	0.74
1:H:228:ASN:OD1	1:H:229:PRO:CG	2.30	0.74
1:B:485:GLY:O	1:B:486:ASN:HB2	1.85	0.74
1:D:362:LEU:HA	1:H:356:ASN:HB3	1.69	0.74
1:F:96:PHE:O	1:F:97:PHE:HB2	1.87	0.74
1:F:147:THR:HA	1:F:171:GLN:HE22	1.53	0.74
1:G:397:GLY:O	1:G:487:ALA:O	2.05	0.74
1:B:379:THR:HG23	1:B:380:THR:N	2.01	0.74
1:F:148:GLN:HE21	1:F:150:ARG:CZ	2.01	0.74
1:G:147:THR:CB	1:G:171:GLN:NE2	2.50	0.74
1:C:213:GLU:O	1:C:214:GLN:CD	2.30	0.74
1:C:277:PRO:HB3	1:C:280:GLY:HA2	1.69	0.74
1:G:194:ASN:HD22	1:G:196:GLY:N	1.86	0.74
1:C:215:ASP:OD1	1:C:215:ASP:C	2.31	0.74
1:D:182:ASP:OD2	1:D:182:ASP:C	2.30	0.74
1:G:400:ASP:OD1	1:G:400:ASP:C	2.30	0.74
1:G:144:ALA:HB1	1:G:145:ASN:O	1.88	0.73
1:H:194:ASN:HD22	1:H:196:GLY:N	1.85	0.73
1:A:381:GLN:C	1:A:382:THR:OG1	2.30	0.73
1:F:4:GLU:OE2	1:F:4:GLU:C	2.31	0.73
1:G:243:GLY:C	1:G:253:PHE:HE1	1.95	0.73
1:B:98:ASN:HB2	1:B:100:THR:HG22	1.69	0.73
1:C:378:ASN:O	1:C:379:THR:CG2	2.29	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:ASN:HD22	1:E:196:GLY:N	1.85	0.73
1:H:121:GLN:HG3	1:H:149:PHE:HE2	1.52	0.73
1:A:212:THR:HG22	1:A:215:ASP:C	2.14	0.73
1:B:136:TYR:CE1	1:B:184:LYS:HD3	2.24	0.73
1:F:192:PHE:CD2	1:F:193:ALA:CB	2.69	0.73
1:H:97:PHE:CE2	1:H:106:ARG:CG	2.69	0.73
1:A:277:PRO:HB3	1:A:280:GLY:HA2	1.69	0.73
1:D:98:ASN:HB2	1:D:100:THR:HG22	1.71	0.73
1:F:194:ASN:HD22	1:F:196:GLY:N	1.85	0.73
1:A:422:ASN:CA	1:A:423:SER:HB2	2.17	0.73
1:A:213:GLU:C	1:A:214:GLN:CD	2.50	0.73
1:D:213:GLU:C	1:D:214:GLN:CD	2.49	0.73
1:H:486:ASN:CA	1:H:487:ALA:HB2	2.08	0.73
1:F:147:THR:CB	1:F:171:GLN:HE21	2.01	0.73
1:A:31:LYS:HB3	1:A:104:ARG:HE	1.54	0.73
1:G:497:VAL:CG2	1:G:497:VAL:O	2.36	0.72
1:A:212:THR:CG2	1:A:215:ASP:O	2.36	0.72
1:A:352:LEU:CD1	1:A:503:ILE:CG1	2.66	0.72
1:A:379:THR:HG21	1:A:450:ASP:O	1.87	0.72
1:H:147:THR:HA	1:H:171:GLN:HE22	1.53	0.72
1:B:353:THR:HB	1:B:498:ASP:OD2	1.88	0.72
1:E:231:ALA:HB3	1:E:232:PRO:HD3	1.70	0.72
1:F:229:PRO:HG2	1:F:230:GLY:H	1.53	0.72
1:H:400:ASP:O	1:H:401:PRO:O	2.07	0.72
1:C:213:GLU:O	1:C:214:GLN:HG2	1.88	0.72
1:E:147:THR:HA	1:E:171:GLN:HE22	1.53	0.72
1:F:497:VAL:CG1	1:F:497:VAL:O	2.38	0.72
1:H:400:ASP:OD1	1:H:401:PRO:O	2.08	0.72
1:A:98:ASN:HB2	1:A:100:THR:HG22	1.71	0.72
1:C:380:THR:O	1:C:380:THR:CG2	2.35	0.72
1:D:321:ASN:HB2	1:D:322:PRO:HD2	1.72	0.72
1:H:98:ASN:ND2	1:H:98:ASN:H	1.88	0.72
1:B:31:LYS:HB3	1:B:104:ARG:HE	1.55	0.72
1:D:212:THR:HG23	1:D:213:GLU:O	1.90	0.72
1:H:383:ILE:O	1:H:384:SER:HB2	1.88	0.72
1:B:448:GLU:O	1:B:449:ASN:CG	2.32	0.72
1:C:255:ASN:O	1:D:194:ASN:O	2.08	0.72
1:D:192:PHE:CD2	1:D:192:PHE:O	2.43	0.72
1:E:232:PRO:HG2	1:F:441:ASN:HB2	1.71	0.71
1:D:424:LYS:C	1:D:425:VAL:HG23	2.15	0.71
1:D:192:PHE:HA	1:D:193:ALA:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:SER:CB	1:D:185:SER:O	2.32	0.71
1:G:346:PHE:CE1	1:G:360:VAL:CG2	2.73	0.71
1:G:353:THR:HA	1:G:498:ASP:O	1.91	0.71
1:A:422:ASN:CA	1:A:423:SER:CB	2.68	0.71
1:E:5:THR:O	1:E:6:SER:HB2	1.91	0.71
1:E:147:THR:CB	1:E:171:GLN:HE21	2.01	0.71
1:G:398:LEU:N	1:G:487:ALA:O	2.24	0.71
1:A:195:GLU:OE2	1:A:195:GLU:CA	2.38	0.71
1:G:148:GLN:HE21	1:G:150:ARG:CZ	2.03	0.71
1:H:147:THR:CB	1:H:171:GLN:HE21	2.01	0.71
1:H:423:SER:OG	1:H:425:VAL:HG23	1.91	0.71
1:C:171:GLN:HE21	1:D:323:GLU:HG2	1.55	0.71
1:E:228:ASN:HD21	1:E:229:PRO:HB3	1.49	0.71
1:G:229:PRO:CG	1:G:230:GLY:H	2.02	0.70
1:F:121:GLN:HG3	1:F:149:PHE:HE2	1.54	0.70
1:G:147:THR:CB	1:G:171:GLN:HE21	2.04	0.70
1:G:401:PRO:O	1:G:402:GLU:CB	2.38	0.70
1:H:96:PHE:CB	1:H:97:PHE:HD1	2.04	0.70
1:A:352:LEU:HD11	1:A:503:ILE:CG1	2.22	0.70
1:F:5:THR:O	1:F:300:ASN:O	2.10	0.70
1:F:144:ALA:CB	1:F:145:ASN:CA	2.67	0.70
1:D:31:LYS:HB3	1:D:104:ARG:HE	1.56	0.70
1:F:231:ALA:HB3	1:F:232:PRO:HD3	1.73	0.70
1:B:378:ASN:ND2	1:B:380:THR:O	2.23	0.70
1:D:395:PHE:CE2	1:D:407:MET:HE2	2.26	0.70
1:E:121:GLN:HG3	1:E:149:PHE:HE2	1.54	0.70
1:G:318:TYR:CD2	1:G:319:GLN:O	2.45	0.70
1:H:148:GLN:HE21	1:H:150:ARG:CZ	2.03	0.70
1:C:31:LYS:HB3	1:C:104:ARG:HE	1.55	0.70
1:G:194:ASN:CA	1:G:195:GLU:CB	2.49	0.70
1:F:298:PRO:HD3	1:F:427:PHE:CD2	2.26	0.70
1:B:346:PHE:CE1	1:B:360:VAL:HG23	2.26	0.70
1:F:397:GLY:O	1:F:487:ALA:C	2.35	0.70
1:G:144:ALA:CB	1:G:145:ASN:CA	2.67	0.70
1:F:4:GLU:N	1:F:4:GLU:OE2	2.25	0.69
1:F:318:TYR:CD2	1:F:319:GLN:O	2.45	0.69
1:F:397:GLY:HA2	1:F:400:ASP:O	1.91	0.69
1:A:381:GLN:O	1:A:382:THR:OG1	2.09	0.69
1:D:195:GLU:HB3	1:D:241:PHE:CZ	2.27	0.69
1:H:318:TYR:CD2	1:H:319:GLN:O	2.45	0.69
1:H:401:PRO:C	1:H:403:GLU:H	2.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLU:OE2	1:A:195:GLU:HA	1.91	0.69
1:B:403:GLU:OE2	1:B:424:LYS:HG3	1.92	0.69
1:G:62:LEU:HD22	1:G:309:VAL:HG21	1.74	0.69
1:A:213:GLU:O	1:A:214:GLN:OE1	2.02	0.69
1:B:383:ILE:O	1:B:384:SER:CB	2.41	0.69
1:D:385:LYS:HG3	1:D:386:SER:N	2.05	0.69
1:F:486:ASN:CA	1:F:487:ALA:CB	2.55	0.69
1:G:229:PRO:HG2	1:G:230:GLY:H	1.58	0.69
1:A:195:GLU:HB3	1:A:241:PHE:CZ	2.28	0.69
1:A:395:PHE:CE2	1:A:407:MET:HE2	2.28	0.69
1:C:346:PHE:CE1	1:C:360:VAL:HG23	2.28	0.69
1:F:96:PHE:O	1:F:97:PHE:CB	2.41	0.69
1:F:397:GLY:C	1:F:487:ALA:O	2.36	0.69
1:G:5:THR:O	1:G:6:SER:CB	2.40	0.69
1:G:256:GLN:NE2	1:G:326:LEU:HB2	2.07	0.69
1:C:98:ASN:HB2	1:C:100:THR:HG22	1.73	0.69
1:H:194:ASN:CA	1:H:195:GLU:CB	2.48	0.69
1:D:346:PHE:CE1	1:D:360:VAL:HG23	2.28	0.68
1:E:194:ASN:ND2	1:E:196:GLY:N	2.41	0.68
1:F:62:LEU:HD22	1:F:309:VAL:HG21	1.73	0.68
1:A:277:PRO:HA	1:A:278:THR:C	2.19	0.68
1:D:192:PHE:CE1	1:D:195:GLU:CG	2.77	0.68
1:G:144:ALA:CB	1:G:145:ASN:HA	2.22	0.68
1:G:411:VAL:HG21	1:G:500:LEU:CD2	2.23	0.68
1:G:427:PHE:O	1:G:427:PHE:CD2	2.45	0.68
1:H:497:VAL:CG1	1:H:497:VAL:O	2.42	0.68
1:C:321:ASN:HB2	1:C:322:PRO:HD2	1.76	0.68
1:E:318:TYR:CD2	1:E:319:GLN:O	2.45	0.68
1:G:243:GLY:C	1:G:253:PHE:CE1	2.70	0.68
1:A:346:PHE:CE1	1:A:360:VAL:HG23	2.29	0.68
1:C:192:PHE:HA	1:C:193:ALA:HB2	1.76	0.68
1:D:192:PHE:CZ	1:D:195:GLU:CG	2.77	0.68
1:D:423:SER:O	1:D:425:VAL:HG23	1.94	0.68
1:E:4:GLU:CG	1:E:4:GLU:O	2.42	0.68
1:A:323:GLU:HG2	1:B:171:GLN:HE21	1.56	0.68
1:B:192:PHE:CD2	1:B:192:PHE:C	2.71	0.68
1:B:183:LEU:HD23	1:B:186:TRP:HZ2	1.59	0.68
1:F:98:ASN:N	1:F:98:ASN:ND2	2.41	0.68
1:F:496:GLY:O	1:F:497:VAL:HB	1.92	0.68
1:G:228:ASN:HD21	1:G:229:PRO:HG3	1.53	0.68
1:G:397:GLY:C	1:G:487:ALA:O	2.37	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:346:PHE:HE1	1:H:360:VAL:HG23	1.58	0.68
1:A:352:LEU:HD13	1:A:503:ILE:HG12	1.73	0.68
1:C:195:GLU:HB3	1:C:241:PHE:CZ	2.28	0.68
1:C:214:GLN:HG2	1:C:215:ASP:N	2.06	0.68
1:E:228:ASN:OD1	1:E:229:PRO:HB3	1.90	0.68
1:E:298:PRO:HD3	1:E:427:PHE:HD2	1.58	0.68
1:F:141:VAL:HG23	1:F:186:TRP:CD1	2.29	0.68
1:A:398:LEU:CB	1:A:487:ALA:CB	2.65	0.67
1:E:395:PHE:HE2	1:E:407:MET:HE2	1.59	0.67
1:D:175:ILE:HD13	1:D:205:PRO:HB3	1.75	0.67
1:D:213:GLU:O	1:D:214:GLN:CG	2.42	0.67
1:E:395:PHE:HB3	1:E:488:LEU:HB3	1.75	0.67
1:F:277:PRO:HA	1:F:278:THR:C	2.19	0.67
1:H:198:LEU:HD12	1:H:198:LEU:O	1.93	0.67
1:B:277:PRO:HA	1:B:278:THR:C	2.19	0.67
1:E:62:LEU:HD22	1:E:309:VAL:HG21	1.76	0.67
1:G:96:PHE:O	1:G:97:PHE:CD1	2.47	0.67
1:G:98:ASN:N	1:G:98:ASN:ND2	2.30	0.67
1:G:441:ASN:HB2	1:H:232:PRO:CG	2.23	0.67
1:H:62:LEU:HD22	1:H:309:VAL:HG21	1.75	0.67
1:E:98:ASN:N	1:E:98:ASN:HD22	1.91	0.67
1:F:228:ASN:OD1	1:F:229:PRO:HG3	1.94	0.67
1:F:401:PRO:C	1:F:403:GLU:H	2.02	0.67
1:H:141:VAL:HG23	1:H:186:TRP:CD1	2.29	0.67
1:H:228:ASN:HD22	1:H:229:PRO:HB3	1.54	0.67
1:C:497:VAL:O	1:C:497:VAL:HG23	1.94	0.67
1:E:198:LEU:HD12	1:E:198:LEU:O	1.95	0.67
1:H:96:PHE:CB	1:H:97:PHE:CD1	2.77	0.67
1:H:97:PHE:CE2	1:H:106:ARG:HG2	2.30	0.67
1:A:182:ASP:O	1:A:183:LEU:HB2	1.93	0.67
1:A:321:ASN:HB2	1:A:322:PRO:HD2	1.75	0.67
1:A:421:GLY:O	1:A:422:ASN:HB2	1.94	0.67
1:E:401:PRO:C	1:E:403:GLU:H	2.02	0.67
1:H:346:PHE:CE1	1:H:360:VAL:CG2	2.78	0.67
1:A:213:GLU:O	1:A:214:GLN:CG	2.43	0.67
1:D:424:LYS:O	1:D:425:VAL:C	2.37	0.67
1:C:212:THR:HG22	1:C:213:GLU:O	1.95	0.67
1:D:449:ASN:O	1:D:449:ASN:ND2	2.28	0.67
1:F:141:VAL:HG21	1:F:186:TRP:HE1	1.60	0.67
1:C:183:LEU:HD23	1:C:186:TRP:CZ2	2.30	0.67
1:C:378:ASN:HA	1:C:451:LEU:CD2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:PHE:O	1:E:97:PHE:HB2	1.94	0.67
1:E:141:VAL:HG23	1:E:186:TRP:CD1	2.30	0.66
1:F:427:PHE:O	1:F:427:PHE:CG	2.48	0.66
1:A:496:GLY:O	1:A:497:VAL:CB	2.43	0.66
1:C:277:PRO:HA	1:C:278:THR:C	2.20	0.66
1:A:192:PHE:HA	1:A:193:ALA:HB2	1.76	0.66
1:E:277:PRO:HA	1:E:278:THR:C	2.19	0.66
1:F:92:ASN:OD1	1:F:96:PHE:O	2.14	0.66
1:F:148:GLN:NE2	1:F:150:ARG:CZ	2.58	0.66
1:F:194:ASN:CA	1:F:195:GLU:CB	2.48	0.66
1:D:463:ASN:OD1	1:D:463:ASN:C	2.39	0.66
1:G:141:VAL:HG23	1:G:186:TRP:CD1	2.30	0.66
1:G:231:ALA:N	1:G:232:PRO:HD2	2.10	0.66
1:B:321:ASN:HB2	1:B:322:PRO:HD2	1.76	0.66
1:C:175:ILE:HD13	1:C:205:PRO:HB3	1.76	0.66
1:D:422:ASN:HA	1:D:423:SER:CB	2.26	0.66
1:H:464:ILE:HG13	1:H:479:THR:HG22	1.76	0.66
1:D:499:ASN:OD1	1:D:499:ASN:C	2.37	0.66
1:B:175:ILE:HD13	1:B:205:PRO:HB3	1.77	0.66
1:C:378:ASN:C	1:C:378:ASN:ND2	2.46	0.66
1:E:254:ASP:O	1:E:255:ASN:HB2	1.95	0.66
1:F:198:LEU:HD12	1:F:198:LEU:O	1.96	0.66
1:A:378:ASN:O	1:A:378:ASN:ND2	2.29	0.66
1:F:194:ASN:ND2	1:F:196:GLY:N	2.41	0.66
1:G:194:ASN:HA	1:G:195:GLU:HB2	1.75	0.66
1:D:136:TYR:CE1	1:D:184:LYS:HD3	2.31	0.65
1:D:277:PRO:HA	1:D:278:THR:C	2.22	0.65
1:G:277:PRO:HA	1:G:278:THR:C	2.21	0.65
1:B:182:ASP:O	1:B:183:LEU:HB2	1.94	0.65
1:D:381:GLN:C	1:D:382:THR:OG1	2.38	0.65
1:B:213:GLU:HB3	1:B:214:GLN:OE1	1.96	0.65
1:D:192:PHE:CZ	1:D:195:GLU:HG2	2.31	0.65
1:D:398:LEU:HB2	1:D:487:ALA:HB3	1.79	0.65
1:D:449:ASN:O	1:D:450:ASP:HB2	1.95	0.65
1:F:5:THR:HG22	1:F:6:SER:O	1.96	0.65
1:A:175:ILE:HD13	1:A:205:PRO:HB3	1.79	0.65
1:C:194:ASN:O	1:D:255:ASN:O	2.14	0.65
1:D:496:GLY:O	1:D:497:VAL:CB	2.43	0.65
1:E:441:ASN:HB2	1:F:232:PRO:HG2	1.78	0.65
1:G:144:ALA:CB	1:G:145:ASN:C	2.69	0.65
1:G:194:ASN:ND2	1:G:196:GLY:N	2.41	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:401:PRO:O	1:G:402:GLU:HB3	1.96	0.65
1:F:381:GLN:O	1:F:382:THR:C	2.40	0.65
1:G:380:THR:HG23	1:G:381:GLN:N	2.11	0.65
1:B:395:PHE:CE2	1:B:407:MET:HE2	2.31	0.65
1:D:195:GLU:OE2	1:D:195:GLU:N	2.30	0.65
1:G:98:ASN:H	1:G:98:ASN:ND2	1.82	0.65
1:G:345:ARG:NH1	1:G:507:GLN:NE2	2.45	0.65
1:D:423:SER:OG	1:D:424:LYS:N	2.27	0.65
1:B:195:GLU:N	1:B:195:GLU:OE2	2.30	0.65
1:F:486:ASN:CA	1:F:487:ALA:HB2	2.17	0.65
1:A:497:VAL:CG2	1:A:497:VAL:O	2.44	0.65
1:B:183:LEU:HD23	1:B:186:TRP:CZ2	2.31	0.65
1:B:401:PRO:C	1:B:403:GLU:H	2.04	0.65
1:E:141:VAL:HG21	1:E:186:TRP:HE1	1.61	0.65
1:G:198:LEU:HD12	1:G:198:LEU:O	1.96	0.65
1:B:182:ASP:OD2	1:B:182:ASP:C	2.40	0.64
1:C:395:PHE:CE2	1:C:407:MET:HE2	2.32	0.64
1:E:96:PHE:O	1:E:97:PHE:HD1	1.78	0.64
1:F:398:LEU:HD11	1:F:489:GLY:CA	2.27	0.64
1:H:277:PRO:HA	1:H:278:THR:C	2.22	0.64
1:D:366:THR:O	1:D:462:GLN:NE2	2.18	0.64
1:E:228:ASN:OD1	1:E:229:PRO:CB	2.45	0.64
1:E:398:LEU:H	1:E:398:LEU:HD13	1.60	0.64
1:A:401:PRO:C	1:A:403:GLU:H	2.04	0.64
1:H:96:PHE:O	1:H:97:PHE:HB2	1.98	0.64
1:A:403:GLU:OE2	1:A:424:LYS:HB2	1.96	0.64
1:C:401:PRO:C	1:C:403:GLU:H	2.04	0.64
1:E:381:GLN:O	1:E:382:THR:C	2.40	0.64
1:G:141:VAL:HG21	1:G:186:TRP:HE1	1.62	0.64
1:A:398:LEU:HD13	1:A:487:ALA:CB	2.28	0.64
1:D:62:LEU:HD22	1:D:309:VAL:HG21	1.79	0.64
1:D:401:PRO:C	1:D:403:GLU:H	2.05	0.64
1:F:383:ILE:O	1:F:384:SER:HB2	1.95	0.64
1:H:148:GLN:NE2	1:H:150:ARG:CZ	2.61	0.64
1:H:198:LEU:C	1:H:198:LEU:CD1	2.70	0.64
1:A:195:GLU:OE2	1:A:195:GLU:N	2.31	0.64
1:C:195:GLU:N	1:C:195:GLU:OE2	2.30	0.64
1:G:231:ALA:N	1:G:232:PRO:CD	2.60	0.64
1:A:192:PHE:CZ	1:A:195:GLU:CG	2.81	0.64
1:C:62:LEU:HD22	1:C:309:VAL:HG21	1.78	0.64
1:E:380:THR:HG23	1:E:381:GLN:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:411:VAL:HG21	1:G:500:LEU:HD21	1.79	0.64
1:C:352:LEU:CD1	1:C:352:LEU:N	2.42	0.63
1:E:96:PHE:O	1:E:97:PHE:CB	2.43	0.63
1:G:148:GLN:NE2	1:G:150:ARG:CZ	2.60	0.63
1:H:96:PHE:HB2	1:H:97:PHE:CD1	2.33	0.63
1:H:194:ASN:HA	1:H:195:GLU:HB2	1.74	0.63
1:H:243:GLY:HA2	1:H:253:PHE:CE1	2.34	0.63
1:H:353:THR:HA	1:H:498:ASP:O	1.98	0.63
1:C:193:ALA:HB3	1:C:195:GLU:OE2	1.98	0.63
1:F:463:ASN:C	1:F:463:ASN:OD1	2.41	0.63
1:C:398:LEU:HB2	1:C:487:ALA:HB3	1.79	0.63
1:G:147:THR:CA	1:G:171:GLN:NE2	2.62	0.63
1:G:175:ILE:N	1:G:192:PHE:O	2.31	0.63
1:G:326:LEU:O	1:G:326:LEU:HD13	1.98	0.63
1:B:212:THR:HG22	1:B:213:GLU:O	1.99	0.63
1:D:182:ASP:OD2	1:D:184:LYS:N	2.31	0.63
1:E:86:MET:HE2	1:E:109:ALA:HB2	1.81	0.63
1:H:228:ASN:ND2	1:H:236:SER:OG	2.31	0.63
1:C:378:ASN:O	1:C:378:ASN:ND2	2.31	0.63
1:E:147:THR:CA	1:E:171:GLN:NE2	2.61	0.63
1:H:141:VAL:HG21	1:H:186:TRP:HE1	1.61	0.63
1:F:380:THR:HG23	1:F:381:GLN:N	2.13	0.63
1:D:4:GLU:OE1	1:D:4:GLU:HA	1.99	0.63
1:E:147:THR:CA	1:E:171:GLN:HE22	2.12	0.63
1:E:277:PRO:HB3	1:E:280:GLY:HA2	1.81	0.63
1:H:147:THR:CA	1:H:171:GLN:NE2	2.62	0.62
1:H:326:LEU:HD13	1:H:326:LEU:O	1.99	0.62
1:H:400:ASP:C	1:H:401:PRO:O	2.41	0.62
1:A:62:LEU:HD22	1:A:309:VAL:HG21	1.80	0.62
1:D:180:SER:OG	1:D:183:LEU:N	2.30	0.62
1:F:147:THR:CA	1:F:171:GLN:NE2	2.61	0.62
1:H:426:LYS:CD	1:H:430:GLU:OE2	2.47	0.62
1:A:500:LEU:C	1:A:500:LEU:CD1	2.72	0.62
1:H:231:ALA:N	1:H:232:PRO:HD2	2.13	0.62
1:D:238:ASN:ND2	1:D:269:LEU:H	1.98	0.62
1:D:425:VAL:O	1:D:426:LYS:C	2.43	0.62
1:D:425:VAL:HG21	1:D:481:PHE:O	2.00	0.62
1:E:385:LYS:HG3	1:E:386:SER:H	1.64	0.62
1:A:4:GLU:HA	1:A:4:GLU:OE1	2.00	0.62
1:B:4:GLU:OE1	1:B:4:GLU:HA	1.98	0.62
1:B:62:LEU:HD22	1:B:309:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:PHE:C	1:C:427:PHE:CD2	2.77	0.62
1:E:96:PHE:C	1:E:97:PHE:CD1	2.78	0.62
1:F:229:PRO:CG	1:F:230:GLY:H	2.11	0.62
1:A:379:THR:CG2	1:A:380:THR:H	2.11	0.62
1:A:383:ILE:O	1:A:384:SER:CB	2.48	0.62
1:C:381:GLN:C	1:C:382:THR:OG1	2.41	0.62
1:E:326:LEU:HD13	1:E:326:LEU:O	2.00	0.62
1:F:198:LEU:C	1:F:198:LEU:CD1	2.73	0.62
1:F:326:LEU:HD13	1:F:326:LEU:O	2.00	0.62
1:G:228:ASN:OD1	1:G:229:PRO:CD	2.48	0.62
1:G:401:PRO:C	1:G:403:GLU:H	2.05	0.62
1:A:343:TRP:CE3	1:A:507:GLN:HB3	2.34	0.62
1:A:381:GLN:C	1:A:383:ILE:H	2.07	0.62
1:G:398:LEU:HD21	1:G:489:GLY:HA3	1.81	0.62
1:G:253:PHE:N	1:G:253:PHE:HD1	1.98	0.62
1:A:396:LYS:HE2	2:A:602:HOH:O	1.99	0.62
1:B:497:VAL:O	1:B:497:VAL:CG2	2.48	0.62
1:F:228:ASN:HD21	1:F:229:PRO:HB3	1.55	0.62
1:F:277:PRO:HB3	1:F:280:GLY:HA2	1.82	0.62
1:G:323:GLU:OE2	1:G:323:GLU:CA	2.48	0.62
1:H:228:ASN:CG	1:H:229:PRO:CB	2.71	0.62
1:H:496:GLY:O	1:H:497:VAL:HG12	2.00	0.62
1:B:195:GLU:OE2	1:B:195:GLU:CA	2.48	0.61
1:B:343:TRP:CE3	1:B:507:GLN:HB3	2.36	0.61
1:C:238:ASN:ND2	1:C:269:LEU:H	1.96	0.61
1:C:323:GLU:HG2	1:D:171:GLN:NE2	2.15	0.61
1:E:323:GLU:OE2	1:E:323:GLU:CA	2.48	0.61
1:F:86:MET:HE2	1:F:109:ALA:HB2	1.82	0.61
1:H:354:LYS:HA	1:H:495:THR:O	2.00	0.61
1:F:147:THR:CA	1:F:171:GLN:HE22	2.13	0.61
1:F:326:LEU:N	1:F:326:LEU:CD1	2.63	0.61
1:A:352:LEU:HD11	1:A:503:ILE:HG13	1.80	0.61
1:A:497:VAL:O	1:A:497:VAL:HG23	2.00	0.61
1:C:4:GLU:HA	1:C:4:GLU:OE1	1.99	0.61
1:E:326:LEU:N	1:E:326:LEU:CD1	2.62	0.61
1:G:228:ASN:HD22	1:G:229:PRO:HB3	1.64	0.61
1:B:192:PHE:HA	1:B:193:ALA:HB2	1.82	0.61
1:F:383:ILE:O	1:F:384:SER:CB	2.47	0.61
1:H:326:LEU:N	1:H:326:LEU:CD1	2.64	0.61
1:F:497:VAL:O	1:F:497:VAL:HG13	1.99	0.61
1:G:147:THR:CA	1:G:171:GLN:HE22	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ILE:N	1:C:383:ILE:HD13	2.16	0.61
1:C:424:LYS:O	1:C:425:VAL:C	2.42	0.61
1:F:194:ASN:HA	1:F:195:GLU:HB2	1.73	0.61
1:H:194:ASN:ND2	1:H:196:GLY:N	2.41	0.61
1:A:448:GLU:O	1:A:449:ASN:CG	2.44	0.61
1:C:448:GLU:OE1	1:C:448:GLU:CA	2.42	0.61
1:F:99:ASP:OD1	1:F:99:ASP:N	2.30	0.61
1:B:86:MET:HE2	1:B:109:ALA:HB2	1.83	0.61
1:E:231:ALA:N	1:E:232:PRO:CD	2.64	0.61
1:G:496:GLY:C	1:G:497:VAL:CG1	2.74	0.61
1:H:380:THR:HG23	1:H:381:GLN:N	2.15	0.61
1:B:496:GLY:C	1:B:497:VAL:HG22	2.25	0.61
1:G:115:THR:HG22	1:G:117:GLU:H	1.66	0.61
1:G:326:LEU:N	1:G:326:LEU:CD1	2.64	0.61
1:A:194:ASN:O	1:B:255:ASN:O	2.19	0.60
1:D:379:THR:CG2	1:D:380:THR:H	2.12	0.60
1:F:4:GLU:OE2	1:F:4:GLU:CA	2.48	0.60
1:H:147:THR:CA	1:H:171:GLN:HE22	2.14	0.60
1:A:36:HIS:HD2	1:A:56:HIS:NE2	1.98	0.60
1:B:238:ASN:ND2	1:B:269:LEU:H	1.96	0.60
1:D:86:MET:HE2	1:D:109:ALA:HB2	1.81	0.60
1:F:98:ASN:N	1:F:98:ASN:HD22	1.99	0.60
1:F:395:PHE:CE2	1:F:407:MET:HE2	2.34	0.60
1:A:192:PHE:CE2	1:A:195:GLU:HG2	2.36	0.60
1:A:238:ASN:ND2	1:A:269:LEU:H	1.98	0.60
1:F:398:LEU:CD1	1:F:489:GLY:H	2.14	0.60
1:G:228:ASN:OD1	1:G:229:PRO:HD3	2.00	0.60
1:G:400:ASP:OD2	1:G:424:LYS:NZ	2.35	0.60
1:H:346:PHE:HE1	1:H:360:VAL:CG2	2.14	0.60
1:F:115:THR:HG22	1:F:117:GLU:H	1.67	0.60
1:A:171:GLN:NE2	1:B:323:GLU:HG2	2.15	0.60
1:E:326:LEU:H	1:E:326:LEU:CD1	2.12	0.60
1:G:398:LEU:CD2	1:G:489:GLY:HA3	2.32	0.60
1:H:277:PRO:HB3	1:H:280:GLY:HA2	1.82	0.60
1:G:198:LEU:C	1:G:198:LEU:CD1	2.72	0.60
1:C:36:HIS:HD2	1:C:56:HIS:NE2	1.99	0.60
1:G:86:MET:HE2	1:G:109:ALA:HB2	1.84	0.60
1:B:36:HIS:HD2	1:B:56:HIS:NE2	2.00	0.60
1:B:499:ASN:OD1	1:B:499:ASN:C	2.45	0.60
1:C:86:MET:HE2	1:C:109:ALA:HB2	1.83	0.60
1:D:192:PHE:CZ	1:D:195:GLU:HG3	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:441:ASN:HB2	1:F:232:PRO:CG	2.32	0.60
1:H:141:VAL:HG23	1:H:186:TRP:HD1	1.67	0.60
1:A:398:LEU:HB3	1:A:487:ALA:HB3	1.80	0.59
1:C:343:TRP:CE3	1:C:507:GLN:HB3	2.36	0.59
1:D:343:TRP:CE3	1:D:507:GLN:HB3	2.37	0.59
1:E:115:THR:HG22	1:E:117:GLU:H	1.67	0.59
1:F:398:LEU:N	1:F:487:ALA:O	2.34	0.59
1:E:175:ILE:N	1:E:192:PHE:O	2.33	0.59
1:H:400:ASP:OD1	1:H:400:ASP:C	2.45	0.59
1:A:395:PHE:HE2	1:A:407:MET:HE2	1.65	0.59
1:F:321:ASN:C	1:F:323:GLU:N	2.60	0.59
1:G:98:ASN:C	1:G:100:THR:H	2.08	0.59
1:H:115:THR:HG22	1:H:117:GLU:H	1.67	0.59
1:A:86:MET:HE2	1:A:109:ALA:HB2	1.85	0.59
1:F:141:VAL:HG23	1:F:186:TRP:HD1	1.67	0.59
1:H:323:GLU:OE2	1:H:323:GLU:CA	2.48	0.59
1:F:385:LYS:CG	1:F:386:SER:N	2.62	0.59
1:G:277:PRO:HB3	1:G:280:GLY:HA2	1.83	0.59
1:A:196:GLY:HA2	1:A:197:PHE:C	2.28	0.59
1:E:198:LEU:C	1:E:198:LEU:CD1	2.72	0.59
1:F:231:ALA:N	1:F:232:PRO:HD2	2.17	0.59
1:F:346:PHE:CE1	1:F:360:VAL:HG23	2.38	0.59
1:G:253:PHE:CD1	1:G:253:PHE:N	2.70	0.59
1:H:321:ASN:C	1:H:323:GLU:N	2.61	0.59
1:D:395:PHE:HE2	1:D:407:MET:HE2	1.66	0.59
1:B:381:GLN:C	1:B:382:THR:OG1	2.46	0.59
1:F:98:ASN:ND2	1:F:98:ASN:H	2.00	0.59
1:A:183:LEU:HD23	1:A:186:TRP:HZ2	1.68	0.59
1:D:460:LEU:HG	1:D:465:LEU:HD12	1.85	0.59
1:B:398:LEU:HB2	1:B:487:ALA:HB3	1.84	0.58
1:D:36:HIS:HD2	1:D:56:HIS:NE2	2.00	0.58
1:A:213:GLU:CB	1:A:214:GLN:OE1	2.50	0.58
1:A:423:SER:OG	1:A:424:LYS:N	2.36	0.58
1:E:194:ASN:HA	1:E:195:GLU:HB2	1.74	0.58
1:F:148:GLN:HE21	1:F:150:ARG:NE	2.00	0.58
1:H:427:PHE:O	1:H:427:PHE:CG	2.55	0.58
1:A:398:LEU:HD12	1:A:489:GLY:HA3	1.86	0.58
1:E:395:PHE:O	1:E:404:TYR:HB2	2.04	0.58
1:G:231:ALA:H	1:G:232:PRO:CD	2.16	0.58
1:G:347:ALA:HB2	1:G:358:TYR:CE1	2.38	0.58
1:H:97:PHE:CD2	1:H:106:ARG:HD3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:228:ASN:HD21	1:H:229:PRO:HG3	1.59	0.58
1:D:196:GLY:HA2	1:D:197:PHE:C	2.28	0.58
1:D:354:LYS:HB3	1:D:498:ASP:OD2	2.04	0.58
1:E:231:ALA:N	1:E:232:PRO:HD2	2.18	0.58
1:A:423:SER:O	1:A:424:LYS:CB	2.36	0.58
1:E:141:VAL:HG23	1:E:186:TRP:HD1	1.68	0.58
1:E:228:ASN:ND2	1:E:236:SER:OG	2.36	0.58
1:E:321:ASN:C	1:E:323:GLU:N	2.62	0.58
1:F:5:THR:O	1:F:6:SER:CB	2.30	0.58
1:F:323:GLU:OE2	1:F:323:GLU:CA	2.48	0.58
1:G:397:GLY:O	1:G:487:ALA:C	2.45	0.58
1:B:196:GLY:HA2	1:B:197:PHE:C	2.28	0.58
1:B:424:LYS:O	1:B:425:VAL:CB	2.49	0.58
1:E:148:GLN:HE21	1:E:150:ARG:CZ	2.16	0.58
1:F:403:GLU:HG2	1:F:482:MET:HG3	1.86	0.58
1:G:98:ASN:C	1:G:100:THR:N	2.62	0.58
1:A:197:PHE:CE1	1:B:258:ARG:HA	2.39	0.58
1:A:212:THR:HG22	1:A:212:THR:O	2.02	0.58
1:B:209:GLU:HG3	1:B:221:TRP:CE2	2.39	0.58
1:C:258:ARG:HA	1:D:197:PHE:CE1	2.39	0.58
1:E:486:ASN:CA	1:E:487:ALA:HB2	2.20	0.58
1:C:398:LEU:HD12	1:C:489:GLY:HA3	1.85	0.57
1:G:298:PRO:HD3	1:G:427:PHE:CD2	2.39	0.57
1:E:346:PHE:CE1	1:E:360:VAL:HG23	2.39	0.57
1:C:379:THR:CG2	1:C:380:THR:H	2.16	0.57
1:G:148:GLN:HE21	1:G:150:ARG:NE	2.02	0.57
1:G:486:ASN:CA	1:G:487:ALA:HB2	2.21	0.57
1:G:497:VAL:HG22	1:G:497:VAL:O	2.04	0.57
1:A:379:THR:HG22	1:A:380:THR:H	1.69	0.57
1:B:381:GLN:O	1:B:383:ILE:N	2.31	0.57
1:C:196:GLY:HA2	1:C:197:PHE:C	2.28	0.57
1:D:192:PHE:CD2	1:D:192:PHE:C	2.82	0.57
1:F:175:ILE:N	1:F:192:PHE:O	2.34	0.57
1:G:426:LYS:O	1:G:430:GLU:HB2	2.05	0.57
1:H:175:ILE:N	1:H:192:PHE:O	2.32	0.57
1:E:403:GLU:HG2	1:E:482:MET:HG3	1.85	0.57
1:H:426:LYS:HD2	1:H:430:GLU:OE2	2.03	0.57
1:D:383:ILE:C	1:D:384:SER:OG	2.47	0.57
1:H:86:MET:HE2	1:H:109:ALA:HB2	1.85	0.57
1:H:148:GLN:HE21	1:H:150:ARG:NE	2.03	0.57
1:A:382:THR:C	1:A:383:ILE:HG12	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:ASN:CG	1:B:450:ASP:H	2.08	0.57
1:D:497:VAL:CG2	1:D:497:VAL:O	2.52	0.57
1:F:145:ASN:N	1:F:146:SER:CA	2.63	0.57
1:F:482:MET:HG2	1:F:488:LEU:HD21	1.87	0.57
1:G:96:PHE:O	1:G:97:PHE:CB	2.52	0.57
1:G:141:VAL:HG23	1:G:186:TRP:HD1	1.69	0.57
1:E:497:VAL:HG11	1:E:500:LEU:CB	2.34	0.56
1:A:209:GLU:HG3	1:A:221:TRP:CE2	2.39	0.56
1:G:387:VAL:HG13	1:G:388:PHE:N	2.19	0.56
1:H:145:ASN:N	1:H:146:SER:CA	2.63	0.56
1:A:449:ASN:CG	1:A:450:ASP:H	2.08	0.56
1:C:258:ARG:NH2	1:C:328:ASN:OD1	2.39	0.56
1:C:378:ASN:HD22	1:C:380:THR:N	2.02	0.56
1:C:448:GLU:HB2	1:C:453:TYR:HE2	1.70	0.56
1:E:148:GLN:H	1:E:171:GLN:NE2	2.02	0.56
1:E:400:ASP:OD1	1:E:401:PRO:O	2.23	0.56
1:G:285:ILE:HD12	1:G:309:VAL:HG22	1.87	0.56
1:G:98:ASN:HB2	1:G:100:THR:HG22	0.73	0.56
1:G:121:GLN:CG	1:G:149:PHE:HE2	2.18	0.56
1:H:497:VAL:O	1:H:497:VAL:HG12	2.05	0.56
1:C:182:ASP:OD2	1:C:184:LYS:HG3	2.05	0.56
1:C:192:PHE:C	1:C:192:PHE:HD2	2.06	0.56
1:G:403:GLU:HG2	1:G:482:MET:HG3	1.87	0.56
1:B:448:GLU:O	1:B:449:ASN:C	2.46	0.56
1:G:96:PHE:O	1:G:97:PHE:HB2	2.06	0.56
1:H:285:ILE:HD12	1:H:309:VAL:HG22	1.88	0.56
1:B:195:GLU:OE2	1:B:195:GLU:HA	2.05	0.56
1:E:383:ILE:O	1:E:384:SER:CB	2.54	0.56
1:H:97:PHE:CD2	1:H:106:ARG:CD	2.89	0.56
1:A:212:THR:CG2	1:A:215:ASP:H	2.19	0.56
1:B:395:PHE:HE2	1:B:407:MET:HE2	1.70	0.56
1:C:378:ASN:HD22	1:C:380:THR:H	1.54	0.56
1:H:98:ASN:HB2	1:H:100:THR:CG2	2.09	0.56
1:H:383:ILE:O	1:H:384:SER:CB	2.52	0.56
1:A:362:LEU:HD23	1:F:356:ASN:ND2	2.20	0.55
1:G:321:ASN:C	1:G:323:GLU:N	2.60	0.55
1:H:96:PHE:O	1:H:97:PHE:CB	2.54	0.55
1:H:253:PHE:N	1:H:253:PHE:CD1	2.73	0.55
1:A:110:ILE:HG13	1:A:123:ILE:HG22	1.88	0.55
1:B:258:ARG:NH2	1:B:328:ASN:OD1	2.40	0.55
1:C:182:ASP:O	1:C:183:LEU:CB	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:PRO:HG2	1:F:230:GLY:N	2.21	0.55
1:D:377:VAL:HG12	1:D:379:THR:N	2.22	0.55
1:D:496:GLY:O	1:D:497:VAL:HG13	2.06	0.55
1:G:396:LYS:HG2	1:G:404:TYR:CB	2.33	0.55
1:H:96:PHE:HB2	1:H:97:PHE:CE1	2.41	0.55
1:E:486:ASN:CA	1:E:487:ALA:CB	2.57	0.55
1:F:398:LEU:CD1	1:F:489:GLY:N	2.70	0.55
1:G:326:LEU:H	1:G:326:LEU:CD1	2.14	0.55
1:C:209:GLU:HG3	1:C:221:TRP:CE2	2.41	0.55
1:H:231:ALA:N	1:H:232:PRO:CD	2.68	0.55
1:C:367:GLY:C	1:C:462:GLN:NE2	2.65	0.55
1:C:396:LYS:HE2	2:C:601:HOH:O	2.06	0.55
1:G:341:GLY:HA2	1:G:509:ARG:HD2	1.89	0.55
1:D:209:GLU:HG3	1:D:221:TRP:CE2	2.42	0.55
1:D:398:LEU:HD12	1:D:489:GLY:HA3	1.88	0.55
1:G:148:GLN:H	1:G:171:GLN:NE2	2.05	0.55
1:B:398:LEU:HD12	1:B:489:GLY:HA3	1.87	0.55
1:F:141:VAL:HG21	1:F:186:TRP:NE1	2.21	0.55
1:F:285:ILE:HD12	1:F:309:VAL:HG22	1.89	0.55
1:H:121:GLN:CG	1:H:149:PHE:HE2	2.18	0.55
1:E:285:ILE:HD12	1:E:309:VAL:HG22	1.88	0.54
1:G:497:VAL:O	1:G:497:VAL:HG23	2.06	0.54
1:H:99:ASP:O	1:H:101:ILE:N	2.40	0.54
1:E:460:LEU:HG	1:E:465:LEU:HD12	1.88	0.54
1:A:27:TRP:CZ2	1:A:107:CYS:SG	3.00	0.54
1:C:383:ILE:HG22	1:C:384:SER:N	2.22	0.54
1:C:395:PHE:HE2	1:C:407:MET:HE2	1.73	0.54
1:E:141:VAL:HG21	1:E:186:TRP:NE1	2.22	0.54
1:H:141:VAL:HG21	1:H:186:TRP:NE1	2.22	0.54
1:A:398:LEU:CD1	1:A:487:ALA:CB	2.85	0.54
1:B:27:TRP:CZ2	1:B:107:CYS:SG	3.00	0.54
1:C:398:LEU:CB	1:C:487:ALA:HB3	2.38	0.54
1:C:425:VAL:HG21	1:C:481:PHE:O	2.07	0.54
1:C:379:THR:HG22	1:C:380:THR:H	1.73	0.54
1:E:96:PHE:HB2	1:E:97:PHE:CE1	2.42	0.54
1:E:482:MET:HG2	1:E:488:LEU:HD21	1.90	0.54
1:F:15:PRO:HG2	1:F:302:TRP:HB2	1.89	0.54
1:F:398:LEU:CD1	1:F:487:ALA:O	2.50	0.54
1:H:399:GLU:CG	1:H:486:ASN:HD22	2.21	0.54
1:F:200:TYR:CD2	1:F:200:TYR:N	2.76	0.54
1:F:229:PRO:CG	1:F:230:GLY:N	2.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:PRO:HG2	1:H:302:TRP:HB2	1.90	0.54
1:C:192:PHE:CD2	1:C:192:PHE:O	2.51	0.54
1:D:424:LYS:C	1:D:425:VAL:CG2	2.81	0.54
1:E:401:PRO:O	1:E:402:GLU:HB3	2.08	0.54
1:H:97:PHE:HE2	1:H:106:ARG:HA	1.73	0.54
1:H:254:ASP:OD1	1:H:254:ASP:N	2.40	0.54
1:H:341:GLY:HA2	1:H:509:ARG:HD2	1.89	0.54
1:H:380:THR:CG2	1:H:381:GLN:N	2.70	0.54
1:H:381:GLN:HA	1:H:381:GLN:NE2	2.23	0.54
1:H:480:TYR:HD1	1:H:482:MET:HE2	1.73	0.54
1:C:110:ILE:HG13	1:C:123:ILE:HG22	1.89	0.54
1:G:120:GLU:HB3	1:G:140:PRO:HB3	1.90	0.54
1:G:380:THR:CG2	1:G:381:GLN:N	2.71	0.53
1:G:499:ASN:OD1	1:G:499:ASN:C	2.51	0.53
1:H:96:PHE:HZ	1:H:136:TYR:CD1	2.26	0.53
1:B:110:ILE:HG13	1:B:123:ILE:HG22	1.89	0.53
1:C:445:PHE:CE1	1:C:446:LYS:CD	2.92	0.53
1:D:182:ASP:O	1:D:183:LEU:CB	2.56	0.53
1:G:482:MET:HG2	1:G:488:LEU:HD21	1.89	0.53
1:H:98:ASN:OD1	1:H:100:THR:HG21	2.07	0.53
1:H:148:GLN:H	1:H:171:GLN:NE2	2.07	0.53
1:H:426:LYS:O	1:H:430:GLU:HB2	2.08	0.53
1:H:395:PHE:HE2	1:H:407:MET:HE2	1.73	0.53
1:H:399:GLU:HG2	1:H:486:ASN:HD22	1.73	0.53
1:B:411:VAL:HG21	1:B:500:LEU:HD21	1.90	0.53
1:C:197:PHE:CE1	1:D:258:ARG:HA	2.43	0.53
1:D:212:THR:CG2	1:D:213:GLU:O	2.55	0.53
1:D:385:LYS:CG	1:D:386:SER:N	2.71	0.53
1:G:394:TRP:HB2	1:G:492:ASN:HB2	1.90	0.53
1:H:213:GLU:C	1:H:215:ASP:H	2.17	0.53
1:H:399:GLU:HG3	1:H:486:ASN:ND2	2.24	0.53
1:C:352:LEU:HD12	1:C:501:PHE:O	2.08	0.53
1:D:213:GLU:HG2	1:D:214:GLN:N	2.23	0.53
1:F:213:GLU:C	1:F:215:ASP:H	2.17	0.53
1:G:354:LYS:H	1:G:498:ASP:HA	1.74	0.53
1:B:182:ASP:O	1:B:183:LEU:CB	2.56	0.53
1:C:214:GLN:NE2	1:C:316:THR:OG1	2.40	0.53
1:C:497:VAL:HG22	1:C:497:VAL:O	2.08	0.53
1:E:15:PRO:HG2	1:E:302:TRP:HB2	1.90	0.53
1:H:482:MET:HG2	1:H:488:LEU:HD21	1.90	0.53
1:A:136:TYR:CE1	1:A:184:LYS:HD3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:THR:CG2	1:A:213:GLU:O	2.50	0.53
1:D:110:ILE:HG13	1:D:123:ILE:HG22	1.89	0.53
1:E:380:THR:CG2	1:E:381:GLN:N	2.72	0.53
1:H:231:ALA:HB3	1:H:232:PRO:CD	2.35	0.53
1:B:213:GLU:C	1:B:214:GLN:OE1	2.52	0.53
1:F:141:VAL:CG2	1:F:186:TRP:CD1	2.91	0.53
1:H:231:ALA:H	1:H:232:PRO:CD	2.21	0.53
1:H:345:ARG:NH1	1:H:507:GLN:NE2	2.57	0.53
1:A:183:LEU:HD23	1:A:186:TRP:CZ2	2.43	0.53
1:A:496:GLY:C	1:A:497:VAL:CG1	2.66	0.53
1:D:383:ILE:O	1:D:384:SER:CB	2.56	0.53
1:H:401:PRO:C	1:H:403:GLU:N	2.67	0.53
1:H:499:ASN:C	1:H:499:ASN:OD1	2.51	0.52
1:B:40:GLN:HE22	1:B:82:PHE:HA	1.74	0.52
1:E:121:GLN:CG	1:E:149:PHE:HE2	2.20	0.52
1:H:380:THR:HB	1:H:450:ASP:HB3	1.90	0.52
1:B:425:VAL:O	1:B:426:LYS:C	2.50	0.52
1:C:448:GLU:HB2	1:C:453:TYR:CE2	2.43	0.52
1:E:96:PHE:C	1:E:97:PHE:CG	2.86	0.52
1:E:341:GLY:HA2	1:E:509:ARG:HD2	1.91	0.52
1:F:121:GLN:CG	1:F:149:PHE:HE2	2.21	0.52
1:G:54:TRP:HB2	1:G:72:ILE:HB	1.92	0.52
1:G:400:ASP:OD1	1:G:401:PRO:O	2.27	0.52
1:H:141:VAL:CG2	1:H:186:TRP:CD1	2.92	0.52
1:H:326:LEU:H	1:H:326:LEU:CD1	2.13	0.52
1:H:383:ILE:HD13	1:H:384:SER:H	1.74	0.52
1:A:86:MET:HG3	1:A:108:VAL:O	2.10	0.52
1:E:213:GLU:C	1:E:215:ASP:H	2.18	0.52
1:E:497:VAL:HG11	1:E:500:LEU:HB3	1.91	0.52
1:F:394:TRP:HB2	1:F:492:ASN:HB2	1.91	0.52
1:G:141:VAL:HG21	1:G:186:TRP:NE1	2.23	0.52
1:H:120:GLU:HB3	1:H:140:PRO:HB3	1.92	0.52
1:B:192:PHE:CZ	1:B:195:GLU:HG3	2.44	0.52
1:C:136:TYR:CE1	1:C:184:LYS:HD3	2.44	0.52
1:F:148:GLN:H	1:F:171:GLN:NE2	2.08	0.52
1:F:376:ALA:HA	1:F:452:SER:O	2.09	0.52
1:F:380:THR:CG2	1:F:381:GLN:N	2.72	0.52
1:G:200:TYR:N	1:G:200:TYR:CD2	2.77	0.52
1:H:200:TYR:N	1:H:200:TYR:CD2	2.78	0.52
1:B:401:PRO:O	1:B:402:GLU:HB3	2.10	0.52
1:B:486:ASN:CB	1:B:487:ALA:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ALA:HB1	1:C:350:THR:OG1	2.10	0.52
1:D:379:THR:HG21	1:D:450:ASP:C	2.34	0.52
1:G:381:GLN:C	1:G:382:THR:OG1	2.51	0.52
1:H:394:TRP:HE1	1:H:494:THR:HB	1.75	0.52
1:C:463:ASN:C	1:C:463:ASN:OD1	2.53	0.52
1:E:144:ALA:CB	1:E:145:ASN:C	2.81	0.52
1:G:348:THR:O	1:G:349:ASN:C	2.52	0.52
1:C:486:ASN:CB	1:C:487:ALA:HB2	2.40	0.52
1:F:401:PRO:O	1:F:402:GLU:HB3	2.10	0.52
1:G:15:PRO:HG2	1:G:302:TRP:HB2	1.90	0.52
1:G:256:GLN:NE2	1:G:326:LEU:CB	2.71	0.52
1:H:394:TRP:HB2	1:H:492:ASN:HB2	1.90	0.52
1:E:354:LYS:H	1:E:498:ASP:HA	1.75	0.52
1:G:321:ASN:C	1:G:323:GLU:H	2.18	0.52
1:H:228:ASN:OD1	1:H:229:PRO:CD	2.58	0.52
1:A:258:ARG:NH2	1:A:328:ASN:OD1	2.40	0.52
1:A:356:ASN:HB3	1:F:362:LEU:HA	1.91	0.52
1:D:398:LEU:CB	1:D:487:ALA:HB3	2.39	0.52
1:E:120:GLU:HB3	1:E:140:PRO:HB3	1.90	0.52
1:E:148:GLN:NE2	1:E:150:ARG:CZ	2.72	0.52
1:G:200:TYR:N	1:G:200:TYR:HD2	2.08	0.52
1:G:213:GLU:C	1:G:215:ASP:H	2.17	0.52
1:H:400:ASP:O	1:H:400:ASP:CG	2.53	0.52
1:F:120:GLU:HB3	1:F:140:PRO:HB3	1.91	0.51
1:B:424:LYS:O	1:B:425:VAL:O	2.27	0.51
1:C:171:GLN:NE2	1:D:323:GLU:HG2	2.24	0.51
1:D:378:ASN:O	1:D:450:ASP:O	2.29	0.51
1:F:175:ILE:HG13	1:F:225:ILE:HD12	1.92	0.51
1:F:326:LEU:H	1:F:326:LEU:CD1	2.13	0.51
1:F:341:GLY:HA2	1:F:509:ARG:HD2	1.91	0.51
1:F:347:ALA:HB2	1:F:358:TYR:CZ	2.45	0.51
1:G:145:ASN:HB3	1:G:147:THR:H	1.75	0.51
1:C:377:VAL:HG12	1:C:379:THR:H	1.75	0.51
1:C:381:GLN:O	1:C:382:THR:OG1	2.29	0.51
1:D:347:ALA:HB1	1:D:350:THR:OG1	2.10	0.51
1:E:347:ALA:HB2	1:E:358:TYR:CZ	2.46	0.51
1:H:144:ALA:CB	1:H:145:ASN:C	2.80	0.51
1:C:383:ILE:HD13	1:C:383:ILE:H	1.74	0.51
1:G:141:VAL:CG2	1:G:186:TRP:CD1	2.93	0.51
1:H:98:ASN:OD1	1:H:100:THR:CG2	2.59	0.51
1:A:182:ASP:O	1:A:183:LEU:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:PHE:O	1:D:192:PHE:HD2	1.94	0.51
1:E:141:VAL:CG2	1:E:186:TRP:CD1	2.92	0.51
1:F:401:PRO:C	1:F:403:GLU:N	2.69	0.51
1:H:144:ALA:HB1	1:H:145:ASN:O	2.11	0.51
1:H:243:GLY:HA2	1:H:253:PHE:CD1	2.45	0.51
1:D:27:TRP:CZ2	1:D:107:CYS:SG	3.03	0.51
1:D:182:ASP:O	1:D:183:LEU:HB2	2.11	0.51
1:E:376:ALA:HA	1:E:452:SER:O	2.10	0.51
1:H:500:LEU:HD12	1:H:500:LEU:O	2.10	0.51
1:D:40:GLN:HE22	1:D:82:PHE:HA	1.75	0.51
1:D:486:ASN:CB	1:D:487:ALA:HB2	2.41	0.51
1:F:54:TRP:HB2	1:F:72:ILE:HB	1.92	0.51
1:F:397:GLY:HA2	1:F:400:ASP:C	2.36	0.51
1:D:321:ASN:HB2	1:D:322:PRO:CD	2.40	0.51
1:C:27:TRP:CZ2	1:C:107:CYS:SG	3.04	0.51
1:E:4:GLU:O	1:E:4:GLU:HG3	2.11	0.51
1:H:348:THR:O	1:H:349:ASN:C	2.54	0.51
1:B:381:GLN:O	1:B:382:THR:OG1	2.28	0.51
1:D:411:VAL:HG21	1:D:500:LEU:HD21	1.93	0.51
1:H:54:TRP:HB2	1:H:72:ILE:HB	1.93	0.51
1:D:192:PHE:CE1	1:D:195:GLU:HG3	2.45	0.50
1:F:200:TYR:N	1:F:200:TYR:HD2	2.08	0.50
1:F:321:ASN:C	1:F:323:GLU:H	2.18	0.50
1:F:398:LEU:CD1	1:F:489:GLY:HA3	2.39	0.50
1:G:230:GLY:O	1:G:235:GLY:HA2	2.10	0.50
1:D:381:GLN:C	1:D:382:THR:HG1	2.14	0.50
1:H:97:PHE:HD2	1:H:106:ARG:CD	2.22	0.50
1:H:175:ILE:HG13	1:H:225:ILE:HD12	1.93	0.50
1:A:258:ARG:HA	1:B:197:PHE:CE1	2.46	0.50
1:B:347:ALA:HB1	1:B:350:THR:OG1	2.12	0.50
1:B:369:LEU:HD12	1:B:460:LEU:HD13	1.94	0.50
1:B:378:ASN:O	1:B:379:THR:CB	2.60	0.50
1:C:377:VAL:O	1:C:451:LEU:HD22	2.11	0.50
1:E:368:THR:HG23	1:E:461:ASP:OD1	2.11	0.50
1:E:391:LEU:O	1:E:408:GLY:HA3	2.11	0.50
1:E:463:ASN:OD1	1:E:463:ASN:C	2.53	0.50
1:D:496:GLY:O	1:D:497:VAL:CG1	2.59	0.50
1:E:145:ASN:N	1:E:146:SER:CA	2.64	0.50
1:F:228:ASN:CG	1:F:229:PRO:CG	2.79	0.50
1:F:231:ALA:N	1:F:232:PRO:CD	2.72	0.50
1:G:391:LEU:O	1:G:408:GLY:HA3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:PRO:O	1:D:402:GLU:HB3	2.11	0.50
1:E:175:ILE:HG13	1:E:225:ILE:HD12	1.93	0.50
1:G:401:PRO:C	1:G:403:GLU:N	2.67	0.50
1:H:401:PRO:O	1:H:402:GLU:HB3	2.12	0.50
1:A:193:ALA:O	1:A:194:ASN:OD1	2.30	0.50
1:B:193:ALA:O	1:B:194:ASN:OD1	2.30	0.50
1:B:383:ILE:O	1:B:384:SER:HB2	2.11	0.50
1:C:212:THR:CG2	1:C:213:GLU:O	2.59	0.50
1:F:231:ALA:HB3	1:F:232:PRO:CD	2.41	0.50
1:G:96:PHE:C	1:G:97:PHE:CG	2.88	0.50
1:B:182:ASP:O	1:B:182:ASP:OD2	2.30	0.50
1:C:193:ALA:O	1:C:194:ASN:OD1	2.30	0.50
1:E:54:TRP:HB2	1:E:72:ILE:HB	1.94	0.50
1:E:154:VAL:HG22	1:E:165:MET:HB2	1.93	0.50
1:E:321:ASN:C	1:E:323:GLU:H	2.20	0.50
1:G:175:ILE:HG13	1:G:225:ILE:HD12	1.93	0.50
1:H:395:PHE:CE2	1:H:407:MET:HE2	2.47	0.50
1:A:362:LEU:HD23	1:F:356:ASN:HD22	1.76	0.50
1:C:382:THR:O	1:C:383:ILE:C	2.55	0.50
1:C:496:GLY:O	1:C:497:VAL:HG13	2.11	0.50
1:F:347:ALA:HB2	1:F:358:TYR:CE1	2.47	0.50
1:H:391:LEU:O	1:H:408:GLY:HA3	2.12	0.50
1:H:488:LEU:N	1:H:488:LEU:CD2	2.73	0.50
1:A:383:ILE:C	1:A:384:SER:OG	2.55	0.49
1:B:499:ASN:OD1	1:B:499:ASN:O	2.30	0.49
1:E:200:TYR:N	1:E:200:TYR:CD2	2.77	0.49
1:E:394:TRP:HB2	1:E:492:ASN:HB2	1.94	0.49
1:H:321:ASN:C	1:H:323:GLU:H	2.19	0.49
1:C:182:ASP:O	1:C:182:ASP:OD2	2.30	0.49
1:D:192:PHE:CE1	1:D:195:GLU:HG2	2.46	0.49
1:D:258:ARG:NH2	1:D:328:ASN:OD1	2.45	0.49
1:F:192:PHE:CD1	1:F:193:ALA:CB	2.91	0.49
1:G:192:PHE:CE2	1:G:193:ALA:CB	2.95	0.49
1:G:376:ALA:HA	1:G:452:SER:O	2.12	0.49
1:H:36:HIS:HD2	1:H:56:HIS:NE2	2.10	0.49
1:A:269:LEU:HD11	1:A:312:PHE:CZ	2.48	0.49
1:H:381:GLN:HA	1:H:381:GLN:HE21	1.77	0.49
1:B:483:THR:HG23	1:B:483:THR:O	2.11	0.49
1:C:195:GLU:OE2	1:C:195:GLU:CA	2.60	0.49
1:D:193:ALA:O	1:D:194:ASN:OD1	2.29	0.49
1:D:426:LYS:O	1:D:427:PHE:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:499:ASN:OD1	1:D:499:ASN:O	2.29	0.49
1:F:154:VAL:HG22	1:F:165:MET:HB2	1.94	0.49
1:H:487:ALA:C	1:H:488:LEU:HD23	2.37	0.49
1:A:40:GLN:HE22	1:A:82:PHE:HA	1.76	0.49
1:C:215:ASP:OD1	1:C:217:SER:N	2.45	0.49
1:C:353:THR:HA	1:C:498:ASP:O	2.12	0.49
1:E:192:PHE:CE2	1:E:193:ALA:CB	2.95	0.49
1:E:200:TYR:N	1:E:200:TYR:HD2	2.09	0.49
1:F:195:GLU:C	1:F:195:GLU:OE1	2.55	0.49
1:G:37:LEU:HD11	1:G:306:MET:HE3	1.95	0.49
1:H:347:ALA:HB2	1:H:358:TYR:CE1	2.47	0.49
1:A:394:TRP:HE1	1:A:494:THR:CB	2.23	0.49
1:C:354:LYS:HA	1:C:495:THR:HG23	1.95	0.49
1:D:355:ALA:O	1:H:363:SER:HB2	2.12	0.49
1:B:398:LEU:CB	1:B:487:ALA:HB3	2.42	0.49
1:E:397:GLY:HA2	1:E:400:ASP:C	2.37	0.49
1:E:398:LEU:HD13	1:E:487:ALA:O	2.05	0.49
1:F:213:GLU:O	1:F:214:GLN:HG2	2.13	0.49
1:G:213:GLU:O	1:G:214:GLN:HG2	2.13	0.49
1:H:200:TYR:N	1:H:200:TYR:HD2	2.10	0.49
1:A:269:LEU:HD11	1:A:312:PHE:HZ	1.77	0.49
1:C:378:ASN:ND2	1:C:380:THR:N	2.61	0.49
1:C:378:ASN:HD21	1:C:380:THR:C	2.18	0.49
1:D:424:LYS:O	1:D:425:VAL:O	2.31	0.49
1:E:499:ASN:OD1	1:E:499:ASN:O	2.30	0.49
1:F:147:THR:O	1:F:148:GLN:C	2.56	0.49
1:H:192:PHE:CE2	1:H:193:ALA:CB	2.96	0.49
1:H:499:ASN:OD1	1:H:499:ASN:O	2.30	0.49
1:E:213:GLU:O	1:E:214:GLN:HG2	2.12	0.49
1:E:398:LEU:N	1:E:487:ALA:O	2.46	0.49
1:G:499:ASN:OD1	1:G:499:ASN:O	2.30	0.49
1:E:144:ALA:CB	1:E:145:ASN:CA	2.66	0.49
1:F:192:PHE:CE2	1:F:193:ALA:CB	2.96	0.49
1:F:426:LYS:O	1:F:430:GLU:HB2	2.12	0.49
1:G:256:GLN:HE22	1:G:326:LEU:CB	2.25	0.49
1:G:389:ALA:O	1:G:410:GLU:HA	2.13	0.49
1:B:422:ASN:CA	1:B:423:SER:HB2	2.35	0.48
1:D:346:PHE:HE1	1:D:360:VAL:HG23	1.78	0.48
1:D:382:THR:O	1:D:384:SER:OG	2.30	0.48
1:E:37:LEU:HD11	1:E:306:MET:HE3	1.94	0.48
1:E:148:GLN:HE21	1:E:150:ARG:NE	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419:ASP:CG	1:E:437:ARG:NH1	2.63	0.48
1:F:388:PHE:CE1	1:F:410:GLU:HG3	2.48	0.48
1:F:440:VAL:O	1:F:441:ASN:HB3	2.13	0.48
1:G:253:PHE:HD1	1:G:253:PHE:H	1.59	0.48
1:C:381:GLN:C	1:C:383:ILE:H	2.21	0.48
1:C:401:PRO:O	1:C:402:GLU:HB3	2.13	0.48
1:C:461:ASP:HB3	1:C:464:ILE:HG22	1.94	0.48
1:A:383:ILE:O	1:A:384:SER:OG	2.30	0.48
1:C:182:ASP:OD2	1:C:182:ASP:C	2.54	0.48
1:D:368:THR:CG2	1:D:461:ASP:OD1	2.62	0.48
1:D:383:ILE:O	1:D:384:SER:OG	2.31	0.48
1:E:98:ASN:N	1:E:98:ASN:ND2	2.54	0.48
1:E:395:PHE:O	1:E:404:TYR:CB	2.61	0.48
1:E:401:PRO:C	1:E:403:GLU:N	2.69	0.48
1:G:36:HIS:HD2	1:G:56:HIS:NE2	2.11	0.48
1:C:364:ASN:OD1	1:E:355:ALA:HB1	2.12	0.48
1:D:483:THR:HG23	1:D:483:THR:O	2.13	0.48
1:E:228:ASN:CG	1:E:229:PRO:CG	2.81	0.48
1:G:149:PHE:HZ	1:G:165:MET:CE	2.27	0.48
1:H:96:PHE:HB3	1:H:97:PHE:HD1	1.79	0.48
1:H:147:THR:O	1:H:148:GLN:C	2.56	0.48
1:H:213:GLU:O	1:H:214:GLN:HG2	2.13	0.48
1:H:400:ASP:O	1:H:400:ASP:OD1	2.31	0.48
1:A:121:GLN:HG3	1:A:165:MET:HE1	1.96	0.48
1:C:425:VAL:O	1:C:426:LYS:C	2.57	0.48
1:E:36:HIS:HD2	1:E:56:HIS:NE2	2.12	0.48
1:E:149:PHE:HZ	1:E:165:MET:CE	2.27	0.48
1:G:427:PHE:O	1:G:428:VAL:CG2	2.59	0.48
1:A:401:PRO:O	1:A:402:GLU:HB3	2.13	0.48
1:C:483:THR:HG23	1:C:483:THR:O	2.13	0.48
1:F:398:LEU:HD11	1:F:489:GLY:N	2.28	0.48
1:G:154:VAL:HG22	1:G:165:MET:HB2	1.95	0.48
1:A:255:ASN:O	1:B:194:ASN:O	2.32	0.48
1:E:144:ALA:HB1	1:E:145:ASN:O	2.12	0.48
1:E:432:PRO:O	1:F:437:ARG:HB3	2.13	0.48
1:F:37:LEU:HD11	1:F:306:MET:HE3	1.94	0.48
1:G:352:LEU:HB3	1:G:495:THR:HG21	1.96	0.48
1:B:269:LEU:HD11	1:B:312:PHE:HZ	1.78	0.48
1:B:378:ASN:O	1:B:380:THR:N	2.39	0.48
1:C:163:TRP:CD1	1:C:183:LEU:HG	2.49	0.48
1:E:347:ALA:HB2	1:E:358:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:GLY:O	1:A:486:ASN:ND2	2.47	0.48
1:B:346:PHE:HE1	1:B:360:VAL:HG23	1.77	0.48
1:C:496:GLY:O	1:C:497:VAL:CB	2.61	0.48
1:D:448:GLU:O	1:D:449:ASN:C	2.56	0.48
1:E:383:ILE:O	1:E:384:SER:HB2	2.14	0.48
1:E:500:LEU:O	1:E:500:LEU:CD1	2.33	0.48
1:H:376:ALA:HA	1:H:452:SER:O	2.13	0.48
1:A:448:GLU:O	1:A:449:ASN:OD1	2.32	0.48
1:B:463:ASN:OD1	1:B:463:ASN:C	2.57	0.48
1:E:403:GLU:HG3	1:E:423:SER:HA	1.96	0.48
1:E:440:VAL:O	1:E:441:ASN:HB3	2.14	0.48
1:F:391:LEU:O	1:F:408:GLY:HA3	2.14	0.48
1:F:394:TRP:NE1	1:F:494:THR:HB	2.18	0.48
1:H:96:PHE:HB3	1:H:97:PHE:CD1	2.48	0.48
1:H:354:LYS:H	1:H:498:ASP:HA	1.78	0.48
1:A:403:GLU:OE2	1:A:424:LYS:HG2	2.08	0.47
1:B:383:ILE:O	1:B:384:SER:OG	2.31	0.47
1:C:424:LYS:C	1:C:425:VAL:HG23	2.37	0.47
1:C:449:ASN:O	1:C:449:ASN:OD1	2.30	0.47
1:D:377:VAL:CG1	1:D:379:THR:H	2.26	0.47
1:E:195:GLU:C	1:E:195:GLU:OE1	2.57	0.47
1:F:36:HIS:HD2	1:F:56:HIS:NE2	2.11	0.47
1:F:486:ASN:CA	1:F:487:ALA:HB3	2.35	0.47
1:G:147:THR:O	1:G:148:GLN:C	2.57	0.47
1:G:347:ALA:CB	1:G:350:THR:HG21	2.44	0.47
1:H:99:ASP:C	1:H:101:ILE:N	2.72	0.47
1:H:464:ILE:O	1:H:464:ILE:CG2	2.61	0.47
1:C:411:VAL:HG21	1:C:500:LEU:HD21	1.96	0.47
1:D:269:LEU:HD11	1:D:312:PHE:CZ	2.49	0.47
1:D:449:ASN:O	1:D:449:ASN:CG	2.52	0.47
1:G:352:LEU:O	1:G:498:ASP:O	2.32	0.47
1:G:397:GLY:HA2	1:G:400:ASP:O	2.14	0.47
1:A:401:PRO:C	1:A:403:GLU:N	2.71	0.47
1:B:86:MET:HG3	1:B:108:VAL:O	2.14	0.47
1:B:269:LEU:HD11	1:B:312:PHE:CZ	2.49	0.47
1:C:269:LEU:HD11	1:C:312:PHE:HZ	1.79	0.47
1:C:377:VAL:HG12	1:C:379:THR:N	2.29	0.47
1:D:269:LEU:HD11	1:D:312:PHE:HZ	1.79	0.47
1:B:226:SER:HB2	1:B:267:TYR:CE1	2.50	0.47
1:C:183:LEU:CD2	1:C:186:TRP:HZ2	2.27	0.47
1:D:86:MET:HG3	1:D:108:VAL:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:GLN:HG3	1:D:165:MET:HE1	1.95	0.47
1:E:96:PHE:O	1:E:97:PHE:CG	2.67	0.47
1:H:97:PHE:HD1	1:H:97:PHE:N	2.13	0.47
1:H:440:VAL:O	1:H:441:ASN:HB3	2.14	0.47
1:C:321:ASN:HB2	1:C:322:PRO:CD	2.43	0.47
1:F:96:PHE:C	1:F:97:PHE:CG	2.92	0.47
1:F:149:PHE:HZ	1:F:165:MET:CE	2.27	0.47
1:G:346:PHE:CE1	1:G:360:VAL:HG22	2.48	0.47
1:H:154:VAL:HG22	1:H:165:MET:HB2	1.96	0.47
1:B:54:TRP:HB2	1:B:72:ILE:HB	1.97	0.47
1:C:378:ASN:HA	1:C:451:LEU:HD21	1.97	0.47
1:E:5:THR:O	1:E:6:SER:OG	2.31	0.47
1:B:369:LEU:CD1	1:B:460:LEU:HD13	2.44	0.47
1:C:205:PRO:HA	1:C:224:PHE:O	2.14	0.47
1:C:378:ASN:ND2	1:C:380:THR:H	2.12	0.47
1:E:192:PHE:CD1	1:E:193:ALA:CB	2.91	0.47
1:E:258:ARG:HH21	1:E:326:LEU:HD21	1.79	0.47
1:G:256:GLN:OE1	1:G:327:ILE:CG1	2.61	0.47
1:G:436:ASN:OD1	1:H:437:ARG:NH1	2.47	0.47
1:H:97:PHE:CD1	1:H:97:PHE:N	2.81	0.47
1:H:228:ASN:CG	1:H:229:PRO:HB3	2.31	0.47
1:H:396:LYS:O	1:H:490:SER:HB3	2.14	0.47
1:A:347:ALA:HB1	1:A:350:THR:OG1	2.15	0.47
1:B:448:GLU:O	1:B:449:ASN:OD1	2.32	0.47
1:C:360:VAL:HG22	1:E:358:TYR:CD1	2.50	0.47
1:C:394:TRP:HE1	1:C:494:THR:CB	2.25	0.47
1:F:383:ILE:H	1:F:383:ILE:HG13	1.44	0.47
1:H:195:GLU:C	1:H:195:GLU:OE1	2.58	0.47
1:A:323:GLU:HG2	1:B:171:GLN:NE2	2.25	0.47
1:E:464:ILE:O	1:E:464:ILE:HG23	2.15	0.47
1:H:37:LEU:HD11	1:H:306:MET:HE3	1.97	0.47
1:H:399:GLU:CG	1:H:486:ASN:ND2	2.78	0.47
1:C:121:GLN:HG3	1:C:165:MET:HE1	1.96	0.47
1:C:226:SER:HB2	1:C:267:TYR:CE1	2.50	0.47
1:E:437:ARG:HD2	1:F:432:PRO:HA	1.96	0.47
1:G:258:ARG:HH21	1:G:326:LEU:HD21	1.79	0.47
1:E:96:PHE:HB2	1:E:97:PHE:CD1	2.50	0.46
1:G:347:ALA:HB1	1:G:350:THR:HG21	1.96	0.46
1:H:228:ASN:OD1	1:H:229:PRO:HD3	2.14	0.46
1:B:121:GLN:HG3	1:B:165:MET:HE1	1.95	0.46
1:C:40:GLN:HE22	1:C:82:PHE:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LEU:HD11	1:C:312:PHE:CZ	2.50	0.46
1:G:346:PHE:HE1	1:G:360:VAL:CG2	2.24	0.46
1:G:388:PHE:CE1	1:G:410:GLU:HG3	2.50	0.46
1:G:400:ASP:OD1	1:G:400:ASP:O	2.32	0.46
1:H:149:PHE:HZ	1:H:165:MET:CE	2.28	0.46
1:H:192:PHE:CD1	1:H:193:ALA:CB	2.92	0.46
1:B:316:THR:HA	1:B:327:ILE:HA	1.96	0.46
1:B:401:PRO:C	1:B:403:GLU:N	2.72	0.46
1:E:497:VAL:CG1	1:E:500:LEU:HB3	2.45	0.46
1:H:381:GLN:O	1:H:382:THR:C	2.58	0.46
1:A:449:ASN:CG	1:A:450:ASP:N	2.67	0.46
1:C:401:PRO:C	1:C:403:GLU:N	2.71	0.46
1:E:228:ASN:HA	1:E:229:PRO:HA	1.58	0.46
1:E:368:THR:CG2	1:E:461:ASP:OD1	2.63	0.46
1:A:226:SER:HB2	1:A:267:TYR:CE1	2.51	0.46
1:B:394:TRP:HE1	1:B:494:THR:CB	2.26	0.46
1:C:385:LYS:CG	1:C:386:SER:H	2.29	0.46
1:D:496:GLY:C	1:D:497:VAL:HG13	2.41	0.46
1:F:144:ALA:CB	1:F:145:ASN:C	2.86	0.46
1:G:403:GLU:HG3	1:G:423:SER:HA	1.97	0.46
1:G:440:VAL:O	1:G:441:ASN:HB3	2.14	0.46
1:G:496:GLY:O	1:G:497:VAL:O	2.33	0.46
1:B:385:LYS:CG	1:B:386:SER:H	2.29	0.46
1:D:213:GLU:CB	1:D:214:GLN:OE1	2.63	0.46
1:D:463:ASN:OD1	1:D:463:ASN:O	2.34	0.46
1:E:147:THR:O	1:E:148:GLN:C	2.58	0.46
1:F:258:ARG:HH21	1:F:326:LEU:HD21	1.81	0.46
1:G:192:PHE:CD1	1:G:193:ALA:CB	2.92	0.46
1:G:389:ALA:HA	1:G:497:VAL:CG1	2.45	0.46
1:H:403:GLU:HG3	1:H:423:SER:HA	1.97	0.46
1:A:205:PRO:HA	1:A:224:PHE:O	2.16	0.46
1:E:428:VAL:HG12	1:E:429:LYS:N	2.30	0.46
1:F:231:ALA:O	1:F:233:ALA:O	2.32	0.46
1:H:371:PHE:CE2	1:H:458:GLY:HA3	2.51	0.46
1:A:385:LYS:CG	1:A:386:SER:H	2.29	0.46
1:B:182:ASP:OD2	1:B:184:LYS:HG3	2.16	0.46
1:D:379:THR:HG22	1:D:380:THR:H	1.79	0.46
1:D:425:VAL:O	1:D:428:VAL:N	2.48	0.46
1:G:98:ASN:CB	1:G:100:THR:CG2	2.55	0.46
1:G:194:ASN:CB	1:G:195:GLU:HB3	2.45	0.46
1:A:371:PHE:CE2	1:A:458:GLY:HA3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:LEU:HA	1:C:451:LEU:HD23	1.80	0.46
1:E:232:PRO:HG2	1:F:441:ASN:CB	2.45	0.46
1:G:377:VAL:HG13	1:G:500:LEU:CD2	2.46	0.46
1:A:382:THR:O	1:A:384:SER:OG	2.31	0.46
1:B:205:PRO:HA	1:B:224:PHE:O	2.16	0.46
1:C:195:GLU:HB3	1:C:241:PHE:CE1	2.51	0.46
1:F:50:THR:HA	1:F:51:PRO:C	2.41	0.46
1:F:386:SER:O	1:F:386:SER:OG	2.32	0.46
1:F:403:GLU:HG3	1:F:423:SER:HA	1.97	0.46
1:G:162:LYS:HD3	1:G:179:SER:HB2	1.98	0.46
1:C:378:ASN:ND2	1:C:380:THR:C	2.73	0.45
1:D:448:GLU:O	1:D:449:ASN:OD1	2.33	0.45
1:C:346:PHE:HB3	1:C:347:ALA:H	1.40	0.45
1:G:145:ASN:HB3	1:G:147:THR:N	2.31	0.45
1:G:195:GLU:OE1	1:G:195:GLU:C	2.59	0.45
1:G:429:LYS:HE2	1:G:429:LYS:HB3	1.68	0.45
1:H:396:LYS:C	1:H:490:SER:HB3	2.41	0.45
1:G:496:GLY:O	1:G:497:VAL:HG13	2.16	0.45
1:A:150:ARG:HH22	1:A:201:GLN:NE2	2.14	0.45
1:A:427:PHE:CZ	1:A:434:PHE:CD1	3.05	0.45
1:B:423:SER:C	1:B:424:LYS:HG2	2.40	0.45
1:D:211:PRO:HA	1:D:219:SER:HB3	1.99	0.45
1:A:351:THR:HG21	1:A:499:ASN:OD1	2.16	0.45
1:A:448:GLU:O	1:A:449:ASN:C	2.59	0.45
1:B:383:ILE:C	1:B:384:SER:OG	2.59	0.45
1:C:383:ILE:HG22	1:C:384:SER:H	1.80	0.45
1:D:183:LEU:O	1:D:183:LEU:HD23	2.17	0.45
1:D:226:SER:HB2	1:D:267:TYR:CE1	2.51	0.45
1:E:321:ASN:HB3	1:E:322:PRO:HD2	1.98	0.45
1:F:398:LEU:HD12	1:F:489:GLY:H	1.82	0.45
1:A:378:ASN:HD22	1:A:380:THR:N	2.15	0.45
1:C:183:LEU:CD2	1:C:186:TRP:CZ2	2.99	0.45
1:E:205:PRO:HA	1:E:224:PHE:O	2.17	0.45
1:F:22:ASP:OD1	1:F:22:ASP:N	2.50	0.45
1:F:497:VAL:HG12	1:F:497:VAL:O	2.16	0.45
1:G:96:PHE:C	1:G:97:PHE:CD1	2.95	0.45
1:H:321:ASN:HB3	1:H:322:PRO:HD2	1.99	0.45
1:C:427:PHE:CD2	1:C:428:VAL:N	2.85	0.45
1:E:395:PHE:O	1:E:404:TYR:HA	2.17	0.45
1:F:397:GLY:HA3	1:F:398:LEU:HA	1.81	0.45
1:H:403:GLU:HG2	1:H:482:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:GLU:HB3	1:D:241:PHE:CE1	2.52	0.45
1:E:162:LYS:HD3	1:E:179:SER:HB2	1.99	0.45
1:F:398:LEU:CD1	1:F:489:GLY:CA	2.94	0.45
1:H:403:GLU:CD	1:H:483:THR:HG1	2.24	0.45
1:C:54:TRP:HB2	1:C:72:ILE:HB	1.99	0.45
1:E:8:ARG:NH2	1:E:16:ASN:O	2.50	0.45
1:F:96:PHE:O	1:F:97:PHE:CD1	2.69	0.45
1:G:228:ASN:CB	1:G:229:PRO:HB3	2.47	0.45
1:H:89:ASP:OD2	1:H:94:SER:OG	2.25	0.45
1:H:229:PRO:CD	1:H:230:GLY:H	2.30	0.45
1:H:400:ASP:O	1:H:401:PRO:C	2.60	0.45
1:B:194:ASN:C	1:B:195:GLU:OE2	2.60	0.44
1:B:448:GLU:C	1:B:449:ASN:CG	2.85	0.44
1:E:148:GLN:N	1:E:171:GLN:NE2	2.65	0.44
1:E:497:VAL:CG1	1:E:500:LEU:CB	2.94	0.44
1:H:121:GLN:CG	1:H:149:PHE:CE2	3.00	0.44
1:A:346:PHE:HE1	1:A:360:VAL:HG23	1.81	0.44
1:G:28:TYR:CE2	1:G:276:ASP:HB2	2.52	0.44
1:G:121:GLN:CG	1:G:149:PHE:CE2	3.00	0.44
1:H:22:ASP:OD1	1:H:22:ASP:N	2.50	0.44
1:H:162:LYS:HD3	1:H:179:SER:HB2	1.99	0.44
1:H:380:THR:HB	1:H:450:ASP:CB	2.47	0.44
1:C:86:MET:HG3	1:C:108:VAL:O	2.17	0.44
1:D:205:PRO:HA	1:D:224:PHE:O	2.17	0.44
1:E:346:PHE:CE1	1:E:360:VAL:CG2	3.01	0.44
1:F:145:ASN:OD1	1:F:145:ASN:O	2.36	0.44
1:F:321:ASN:HB3	1:F:322:PRO:HD2	1.99	0.44
1:G:389:ALA:O	1:G:410:GLU:HG2	2.18	0.44
1:H:253:PHE:N	1:H:253:PHE:HD1	2.13	0.44
1:A:30:GLU:HB3	1:A:104:ARG:HD2	1.99	0.44
1:A:321:ASN:HB2	1:A:322:PRO:CD	2.43	0.44
1:B:213:GLU:O	1:B:215:ASP:N	2.50	0.44
1:B:449:ASN:CG	1:B:450:ASP:N	2.66	0.44
1:C:354:LYS:HA	1:C:495:THR:CG2	2.48	0.44
1:C:422:ASN:HA	1:C:423:SER:CB	2.28	0.44
1:C:496:GLY:O	1:C:497:VAL:O	2.35	0.44
1:F:303:ARG:O	1:F:304:SER:HB2	2.18	0.44
1:G:371:PHE:CE2	1:G:458:GLY:HA3	2.52	0.44
1:H:51:PRO:HB3	1:H:77:ASN:HA	1.99	0.44
1:A:41:TYR:CE2	1:A:43:PRO:HB3	2.53	0.44
1:A:483:THR:HG23	1:A:483:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:THR:HG22	1:F:6:SER:N	2.29	0.44
1:F:28:TYR:CE2	1:F:276:ASP:HB2	2.52	0.44
1:F:346:PHE:CE1	1:F:360:VAL:CG2	3.00	0.44
1:C:258:ARG:HA	1:D:197:PHE:HE1	1.83	0.44
1:C:378:ASN:ND2	1:C:380:THR:O	2.41	0.44
1:G:98:ASN:CG	1:G:100:THR:HG22	2.33	0.44
1:G:228:ASN:CG	1:G:229:PRO:CD	2.89	0.44
1:G:460:LEU:HG	1:G:465:LEU:HD12	2.00	0.44
1:A:484:THR:O	1:A:484:THR:HG22	2.18	0.44
1:E:461:ASP:HB3	1:E:464:ILE:HG22	2.00	0.44
1:G:192:PHE:HZ	1:G:252:ALA:HB2	1.82	0.44
1:A:165:MET:HE3	1:A:167:ALA:HB2	2.00	0.44
1:E:50:THR:HA	1:E:51:PRO:C	2.43	0.44
1:E:394:TRP:NE1	1:E:494:THR:HB	2.21	0.44
1:G:45:ASP:OD1	1:G:46:THR:N	2.47	0.44
1:H:28:TYR:CE2	1:H:276:ASP:HB2	2.52	0.44
1:D:5:THR:OG1	1:D:6:SER:N	2.51	0.44
1:E:28:TYR:CE2	1:E:276:ASP:HB2	2.52	0.44
1:E:371:PHE:CE2	1:E:458:GLY:HA3	2.52	0.44
1:E:98:ASN:HB3	1:E:100:THR:CG2	2.48	0.43
1:E:401:PRO:O	1:E:402:GLU:CB	2.65	0.43
1:F:246:ASN:HD21	1:F:249:HIS:HB2	1.83	0.43
1:G:321:ASN:HB3	1:G:322:PRO:HD2	1.99	0.43
1:A:54:TRP:HB2	1:A:72:ILE:HB	2.00	0.43
1:B:382:THR:O	1:B:383:ILE:HG12	2.17	0.43
1:C:346:PHE:HE1	1:C:360:VAL:HG23	1.81	0.43
1:D:371:PHE:CE2	1:D:458:GLY:HA3	2.52	0.43
1:D:377:VAL:CG1	1:D:378:ASN:N	2.76	0.43
1:D:394:TRP:HE1	1:D:494:THR:CB	2.24	0.43
1:E:194:ASN:CB	1:E:195:GLU:HB3	2.44	0.43
1:E:197:PHE:HB2	1:E:200:TYR:CG	2.53	0.43
1:E:386:SER:O	1:E:386:SER:OG	2.32	0.43
1:G:432:PRO:HA	1:H:437:ARG:HE	1.81	0.43
1:H:145:ASN:HB3	1:H:147:THR:H	1.83	0.43
1:H:403:GLU:OE1	1:H:483:THR:OG1	2.33	0.43
1:A:382:THR:O	1:A:383:ILE:C	2.61	0.43
1:B:378:ASN:HA	1:B:451:LEU:HD23	2.00	0.43
1:C:359:ASN:HB3	1:E:359:ASN:HB3	2.00	0.43
1:G:96:PHE:O	1:G:97:PHE:CG	2.71	0.43
1:G:151:ASP:HB3	1:G:204:CYS:HA	2.00	0.43
1:G:246:ASN:HD21	1:G:249:HIS:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:423:SER:CB	1:G:425:VAL:HG23	2.40	0.43
1:B:165:MET:HE3	1:B:167:ALA:HB2	1.98	0.43
1:B:173:TYR:O	1:B:193:ALA:O	2.36	0.43
1:B:192:PHE:CZ	1:B:195:GLU:CG	3.01	0.43
1:B:486:ASN:CA	1:B:487:ALA:HB2	2.48	0.43
1:F:151:ASP:HB3	1:F:204:CYS:HA	2.00	0.43
1:G:426:LYS:HB2	1:G:426:LYS:HE3	1.94	0.43
1:H:388:PHE:CD2	1:H:390:ASP:HB3	2.53	0.43
1:A:427:PHE:CD2	1:A:427:PHE:C	2.97	0.43
1:C:5:THR:OG1	1:C:6:SER:N	2.52	0.43
1:C:424:LYS:O	1:C:425:VAL:O	2.37	0.43
1:G:22:ASP:OD1	1:G:22:ASP:N	2.51	0.43
1:H:151:ASP:HB3	1:H:204:CYS:HA	2.00	0.43
1:H:258:ARG:HH21	1:H:326:LEU:HD21	1.84	0.43
1:B:212:THR:C	1:B:213:GLU:O	2.56	0.43
1:E:151:ASP:HB3	1:E:204:CYS:HA	2.00	0.43
1:E:238:ASN:HD22	1:E:260:VAL:HG21	1.84	0.43
1:F:354:LYS:HD2	1:F:497:VAL:H	1.82	0.43
1:H:403:GLU:OE2	1:H:483:THR:OG1	2.36	0.43
1:D:54:TRP:HB2	1:D:72:ILE:HB	2.00	0.43
1:E:22:ASP:OD1	1:E:22:ASP:N	2.52	0.43
1:E:497:VAL:HG11	1:E:500:LEU:HB2	2.01	0.43
1:F:162:LYS:HD3	1:F:179:SER:HB2	1.99	0.43
1:F:253:PHE:N	1:F:253:PHE:CD1	2.85	0.43
1:G:210:VAL:HA	1:G:211:PRO:HD2	1.89	0.43
1:H:197:PHE:HB2	1:H:200:TYR:CG	2.54	0.43
1:C:371:PHE:CE2	1:C:458:GLY:HA3	2.54	0.43
1:G:228:ASN:CA	1:G:229:PRO:CB	2.97	0.43
1:B:30:GLU:HB3	1:B:104:ARG:HD2	2.01	0.43
1:E:383:ILE:H	1:E:383:ILE:HG13	1.46	0.43
1:G:51:PRO:HB3	1:G:77:ASN:HA	2.00	0.43
1:G:205:PRO:HA	1:G:224:PHE:O	2.19	0.43
1:H:386:SER:O	1:H:386:SER:OG	2.30	0.43
1:B:5:THR:OG1	1:B:6:SER:N	2.51	0.43
1:D:449:ASN:O	1:D:450:ASP:CB	2.63	0.43
1:E:51:PRO:HB3	1:E:77:ASN:HA	2.01	0.43
1:E:153:LYS:HB3	1:E:166:THR:HG23	2.01	0.43
1:E:349:ASN:HA	1:E:502:TYR:OH	2.19	0.43
1:F:371:PHE:CE2	1:F:458:GLY:HA3	2.54	0.43
1:G:8:ARG:NH2	1:G:15:PRO:O	2.49	0.43
1:G:346:PHE:HE1	1:G:360:VAL:HG22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:394:TRP:NE1	1:G:494:THR:HB	2.19	0.43
1:G:397:GLY:HA3	1:G:398:LEU:HA	1.78	0.43
1:H:50:THR:HA	1:H:51:PRO:C	2.44	0.43
1:H:497:VAL:O	1:H:497:VAL:HG13	2.18	0.43
1:B:15:PRO:HD3	1:B:20:MET:SD	2.59	0.42
1:C:356:ASN:HB3	1:E:362:LEU:HA	2.02	0.42
1:D:30:GLU:HB3	1:D:104:ARG:HD2	2.00	0.42
1:E:321:ASN:CB	1:E:322:PRO:HD2	2.50	0.42
1:F:194:ASN:CB	1:F:195:GLU:HB3	2.44	0.42
1:G:256:GLN:HE22	1:G:326:LEU:HB2	1.76	0.42
1:G:389:ALA:HA	1:G:497:VAL:HG11	2.01	0.42
1:G:428:VAL:HG12	1:G:429:LYS:H	1.81	0.42
1:A:424:LYS:HD3	1:A:424:LYS:HA	1.51	0.42
1:B:383:ILE:HB	1:B:384:SER:H	1.60	0.42
1:E:266:TYR:HE2	1:E:269:LEU:HD12	1.84	0.42
1:F:121:GLN:CG	1:F:149:PHE:CE2	3.02	0.42
1:F:464:ILE:O	1:F:464:ILE:HG23	2.17	0.42
1:G:148:GLN:N	1:G:171:GLN:NE2	2.67	0.42
1:H:99:ASP:O	1:H:100:THR:C	2.62	0.42
1:C:383:ILE:CG2	1:C:384:SER:H	2.32	0.42
1:D:425:VAL:O	1:D:427:PHE:N	2.51	0.42
1:D:466:GLU:HG2	1:D:477:THR:HG23	2.01	0.42
1:F:205:PRO:HA	1:F:224:PHE:O	2.19	0.42
1:G:377:VAL:HG13	1:G:500:LEU:HD23	2.00	0.42
1:H:210:VAL:HA	1:H:211:PRO:HD2	1.89	0.42
1:H:429:LYS:HB3	1:H:429:LYS:HE3	1.45	0.42
1:D:426:LYS:O	1:D:429:LYS:N	2.52	0.42
1:E:210:VAL:HA	1:E:211:PRO:HD2	1.88	0.42
1:G:50:THR:HA	1:G:51:PRO:C	2.44	0.42
1:G:381:GLN:C	1:G:382:THR:HG1	2.27	0.42
1:G:383:ILE:H	1:G:383:ILE:HG13	1.46	0.42
1:C:165:MET:HE3	1:C:167:ALA:HB2	2.02	0.42
1:C:213:GLU:OE1	1:C:330:LYS:CD	2.68	0.42
1:E:377:VAL:HG13	1:E:500:LEU:HD11	2.00	0.42
1:H:205:PRO:HA	1:H:224:PHE:O	2.19	0.42
1:H:229:PRO:HD2	1:H:230:GLY:H	1.85	0.42
1:H:303:ARG:O	1:H:304:SER:HB2	2.19	0.42
1:A:197:PHE:HE1	1:B:258:ARG:HA	1.81	0.42
1:B:394:TRP:HB2	1:B:492:ASN:HB2	2.01	0.42
1:E:190:SER:OG	1:E:191:ALA:N	2.51	0.42
1:E:201:GLN:HB2	1:E:228:ASN:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:PHE:HB2	1:F:200:TYR:CG	2.54	0.42
1:G:347:ALA:HB2	1:G:358:TYR:CZ	2.55	0.42
1:B:321:ASN:HB2	1:B:322:PRO:CD	2.44	0.42
1:C:236:SER:HB2	1:C:267:TYR:CD1	2.55	0.42
1:D:212:THR:HG22	1:D:212:THR:O	2.19	0.42
1:E:441:ASN:CB	1:F:232:PRO:HG2	2.49	0.42
1:F:401:PRO:O	1:F:402:GLU:CB	2.67	0.42
1:H:5:THR:O	1:H:5:THR:HG22	2.19	0.42
1:H:246:ASN:HD21	1:H:249:HIS:HB2	1.84	0.42
1:B:380:THR:HA	1:B:381:GLN:HA	1.36	0.42
1:C:287:TRP:HE1	1:C:304:SER:HB3	1.84	0.42
1:D:394:TRP:NE1	1:D:494:THR:HB	2.27	0.42
1:E:145:ASN:HB3	1:E:147:THR:H	1.84	0.42
1:F:51:PRO:HB3	1:F:77:ASN:HA	2.02	0.42
1:G:386:SER:O	1:G:386:SER:OG	2.36	0.42
1:H:266:TYR:HE2	1:H:269:LEU:HD12	1.84	0.42
1:H:397:GLY:H	1:H:401:PRO:HA	1.83	0.42
1:H:463:ASN:C	1:H:463:ASN:OD1	2.62	0.42
1:B:337:ILE:O	1:B:338:SER:HB3	2.20	0.42
1:C:180:SER:HG	1:C:183:LEU:H	1.60	0.42
1:C:425:VAL:O	1:C:428:VAL:N	2.53	0.42
1:D:337:ILE:O	1:D:338:SER:HB3	2.20	0.42
1:A:466:GLU:HG2	1:A:477:THR:HG23	2.01	0.42
1:D:255:ASN:OD1	1:D:255:ASN:C	2.62	0.42
1:E:385:LYS:CG	1:E:386:SER:N	2.61	0.42
1:F:200:TYR:HD2	1:F:200:TYR:H	1.67	0.42
1:F:266:TYR:HE2	1:F:269:LEU:HD12	1.85	0.42
1:G:425:VAL:HG21	1:G:481:PHE:O	2.20	0.42
1:H:153:LYS:HB3	1:H:166:THR:HG23	2.02	0.42
1:A:378:ASN:O	1:A:450:ASP:O	2.38	0.41
1:A:378:ASN:H	1:A:500:LEU:CD1	2.32	0.41
1:B:28:TYR:CZ	1:B:276:ASP:HB2	2.54	0.41
1:B:355:ALA:O	1:G:363:SER:HB2	2.19	0.41
1:C:30:GLU:HB3	1:C:104:ARG:HD2	2.01	0.41
1:C:378:ASN:HA	1:C:451:LEU:HD23	2.01	0.41
1:D:256:GLN:OE1	1:D:258:ARG:HD2	2.19	0.41
1:G:231:ALA:HB3	1:G:232:PRO:CD	2.46	0.41
1:G:388:PHE:HE2	1:G:390:ASP:HB3	1.79	0.41
1:H:200:TYR:HD2	1:H:200:TYR:H	1.68	0.41
1:A:227:ILE:O	1:A:227:ILE:HG13	2.19	0.41
1:A:337:ILE:O	1:A:338:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:THR:HA	1:A:381:GLN:HA	1.37	0.41
1:B:248:THR:OG1	1:B:249:HIS:HD2	2.04	0.41
1:C:337:ILE:O	1:C:338:SER:HB3	2.20	0.41
1:C:362:LEU:HD23	1:E:356:ASN:ND2	2.35	0.41
1:E:149:PHE:HZ	1:E:165:MET:HE1	1.85	0.41
1:E:368:THR:HA	1:E:460:LEU:O	2.20	0.41
1:G:449:ASN:HB3	1:G:450:ASP:H	1.67	0.41
1:B:448:GLU:O	1:B:450:ASP:N	2.53	0.41
1:C:486:ASN:CA	1:C:487:ALA:HB2	2.50	0.41
1:D:303:ARG:O	1:D:304:SER:HB2	2.20	0.41
1:G:228:ASN:HA	1:G:229:PRO:HB3	2.02	0.41
1:H:310:ARG:HB3	1:H:331:ALA:HB1	2.01	0.41
1:B:192:PHE:HA	1:B:193:ALA:CB	2.47	0.41
1:C:376:ALA:HA	1:C:452:SER:O	2.20	0.41
1:G:399:GLU:HG3	1:G:486:ASN:ND2	2.35	0.41
1:A:142:LEU:HD11	1:A:178:TYR:CD1	2.56	0.41
1:A:394:TRP:NE1	1:A:494:THR:HB	2.26	0.41
1:E:266:TYR:CE2	1:E:269:LEU:HD12	2.55	0.41
1:E:371:PHE:CZ	1:E:407:MET:HE3	2.55	0.41
1:G:321:ASN:CB	1:G:322:PRO:HD2	2.50	0.41
1:A:376:ALA:HA	1:A:452:SER:O	2.20	0.41
1:C:484:THR:O	1:C:485:GLY:C	2.64	0.41
1:D:287:TRP:HE1	1:D:304:SER:HB3	1.86	0.41
1:E:45:ASP:OD1	1:E:46:THR:N	2.48	0.41
1:F:371:PHE:CZ	1:F:407:MET:HE3	2.55	0.41
1:G:197:PHE:HB2	1:G:200:TYR:CG	2.56	0.41
1:G:427:PHE:CD2	1:G:427:PHE:C	2.96	0.41
1:H:321:ASN:CB	1:H:322:PRO:HD2	2.50	0.41
1:A:287:TRP:HE1	1:A:304:SER:HB3	1.86	0.41
1:B:150:ARG:HH22	1:B:201:GLN:NE2	2.18	0.41
1:E:426:LYS:HG2	1:E:430:GLU:OE2	2.20	0.41
1:F:96:PHE:O	1:F:97:PHE:CG	2.73	0.41
1:F:153:LYS:HB3	1:F:166:THR:HG23	2.02	0.41
1:F:321:ASN:CB	1:F:322:PRO:HD2	2.50	0.41
1:F:395:PHE:HB3	1:F:488:LEU:HB3	2.03	0.41
1:G:228:ASN:CA	1:G:229:PRO:HB3	2.51	0.41
1:E:4:GLU:O	1:E:4:GLU:HG2	2.21	0.41
1:G:200:TYR:HD2	1:G:200:TYR:H	1.69	0.41
1:G:345:ARG:HH11	1:G:507:GLN:NE2	2.19	0.41
1:A:213:GLU:CA	1:A:214:GLN:OE1	2.68	0.41
1:A:395:PHE:CE2	1:A:407:MET:CE	3.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:LYS:H	1:B:498:ASP:HA	1.86	0.41
1:B:368:THR:CG2	1:B:461:ASP:OD1	2.69	0.41
1:C:150:ARG:HH22	1:C:201:GLN:NE2	2.19	0.41
1:C:227:ILE:O	1:C:227:ILE:HG13	2.20	0.41
1:C:394:TRP:NE1	1:C:494:THR:HB	2.26	0.41
1:D:366:THR:C	1:D:462:GLN:HE22	2.18	0.41
1:D:401:PRO:O	1:D:402:GLU:CB	2.68	0.41
1:E:437:ARG:HB3	1:F:432:PRO:O	2.21	0.41
1:G:238:ASN:HD22	1:G:260:VAL:HG21	1.85	0.41
1:H:228:ASN:CG	1:H:229:PRO:CD	2.90	0.41
1:H:426:LYS:HG2	1:H:430:GLU:OE2	2.20	0.41
1:A:107:CYS:HB2	1:A:126:SER:HB3	2.02	0.41
1:B:391:LEU:O	1:B:408:GLY:HA3	2.21	0.41
1:B:401:PRO:O	1:B:402:GLU:CB	2.68	0.41
1:C:28:TYR:CZ	1:C:276:ASP:HB2	2.56	0.41
1:C:198:LEU:HD23	1:D:326:LEU:HD11	2.03	0.41
1:E:496:GLY:O	1:E:497:VAL:O	2.39	0.41
1:F:210:VAL:HA	1:F:211:PRO:HD2	1.88	0.41
1:F:310:ARG:HB3	1:F:331:ALA:HB1	2.03	0.41
1:G:153:LYS:HB3	1:G:166:THR:HG23	2.03	0.41
1:H:253:PHE:O	1:H:254:ASP:C	2.63	0.41
1:H:461:ASP:O	1:H:463:ASN:N	2.51	0.41
1:B:371:PHE:CE2	1:B:458:GLY:HA3	2.56	0.40
1:G:144:ALA:CB	1:G:145:ASN:O	2.65	0.40
1:G:144:ALA:CA	1:G:145:ASN:C	2.94	0.40
1:H:8:ARG:NH2	1:H:16:ASN:O	2.50	0.40
1:H:381:GLN:HE21	1:H:381:GLN:CA	2.33	0.40
1:A:5:THR:OG1	1:A:6:SER:N	2.53	0.40
1:A:337:ILE:H	1:A:337:ILE:HD12	1.86	0.40
1:A:398:LEU:HB3	1:A:487:ALA:CB	2.46	0.40
1:B:255:ASN:OD1	1:B:255:ASN:C	2.65	0.40
1:C:422:ASN:CA	1:C:423:SER:HB2	2.32	0.40
1:D:165:MET:HE3	1:D:167:ALA:HB2	2.02	0.40
1:E:303:ARG:O	1:E:304:SER:HB2	2.21	0.40
1:E:397:GLY:HA3	1:E:398:LEU:HA	1.83	0.40
1:F:243:GLY:HA2	1:F:253:PHE:CD1	2.55	0.40
1:F:266:TYR:CE2	1:F:269:LEU:HD12	2.56	0.40
1:F:318:TYR:HE2	1:F:320:ALA:O	2.04	0.40
1:G:266:TYR:HE2	1:G:269:LEU:HD12	1.86	0.40
1:B:236:SER:HB2	1:B:267:TYR:CD1	2.55	0.40
1:D:142:LEU:HD11	1:D:178:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:GLY:HA3	1:D:477:THR:H	1.87	0.40
1:D:377:VAL:HG12	1:D:379:THR:H	1.85	0.40
1:E:232:PRO:CG	1:F:441:ASN:HB2	2.44	0.40
1:E:319:GLN:HB3	1:E:320:ALA:H	1.74	0.40
1:G:149:PHE:HZ	1:G:165:MET:HE1	1.86	0.40
1:H:228:ASN:HA	1:H:229:PRO:HA	1.80	0.40
1:H:266:TYR:CE2	1:H:269:LEU:HD12	2.56	0.40
1:H:397:GLY:HA3	1:H:398:LEU:HA	1.82	0.40
1:A:326:LEU:HD11	1:B:198:LEU:HD23	2.03	0.40
1:B:263:GLY:HA3	1:B:477:THR:H	1.87	0.40
1:C:194:ASN:C	1:C:195:GLU:OE2	2.64	0.40
1:C:213:GLU:OE1	1:C:330:LYS:NZ	2.51	0.40
1:C:466:GLU:HG2	1:C:477:THR:HG23	2.04	0.40
1:D:236:SER:HB2	1:D:267:TYR:CD1	2.56	0.40
1:D:397:GLY:HA3	1:D:398:LEU:HA	1.91	0.40
1:E:310:ARG:HB3	1:E:331:ALA:HB1	2.03	0.40
1:H:115:THR:HB	1:H:118:SER:H	1.87	0.40
1:A:236:SER:HB2	1:A:267:TYR:CD1	2.57	0.40
1:B:107:CYS:HB2	1:B:126:SER:HB3	2.04	0.40
1:D:110:ILE:HD13	1:D:154:VAL:CG1	2.51	0.40
1:D:380:THR:HA	1:D:381:GLN:HA	1.30	0.40
1:G:98:ASN:CG	1:G:100:THR:CG2	2.94	0.40
1:G:318:TYR:HE2	1:G:320:ALA:O	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/512 (99%)	452 (89%)	44 (9%)	11 (2%)	5	24
1	B	507/512 (99%)	448 (88%)	46 (9%)	13 (3%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	507/512 (99%)	448 (88%)	47 (9%)	12 (2%)	4	22
1	D	507/512 (99%)	446 (88%)	48 (10%)	13 (3%)	4	21
1	E	507/512 (99%)	446 (88%)	46 (9%)	15 (3%)	3	18
1	F	507/512 (99%)	447 (88%)	45 (9%)	15 (3%)	3	18
1	G	507/512 (99%)	452 (89%)	41 (8%)	14 (3%)	4	19
1	H	507/512 (99%)	448 (88%)	44 (9%)	15 (3%)	3	18
All	All	4056/4096 (99%)	3587 (88%)	361 (9%)	108 (3%)	4	20

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	SER
1	A	424	LYS
1	D	423	SER
1	E	229	PRO
1	E	487	ALA
1	F	229	PRO
1	F	487	ALA
1	G	229	PRO
1	G	428	VAL
1	G	487	ALA
1	H	100	THR
1	H	229	PRO
1	H	401	PRO
1	H	487	ALA
1	A	497	VAL
1	C	423	SER
1	D	497	VAL
1	E	6	SER
1	E	97	PHE
1	E	195	GLU
1	E	230	GLY
1	E	277	PRO
1	E	384	SER
1	E	428	VAL
1	F	6	SER
1	F	97	PHE
1	F	195	GLU
1	F	230	GLY
1	F	428	VAL

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Mol	Chain	Res	Type
1	F	497	VAL
1	G	6	SER
1	G	97	PHE
1	G	195	GLU
1	H	97	PHE
1	H	195	GLU
1	H	428	VAL
1	A	193	ALA
1	A	277	PRO
1	A	384	SER
1	B	193	ALA
1	B	277	PRO
1	B	383	ILE
1	B	384	SER
1	B	486	ASN
1	B	487	ALA
1	C	193	ALA
1	C	277	PRO
1	C	486	ASN
1	C	487	ALA
1	D	193	ALA
1	D	277	PRO
1	D	384	SER
1	D	486	ASN
1	E	214	GLN
1	E	280	GLY
1	F	214	GLN
1	F	277	PRO
1	F	280	GLY
1	F	384	SER
1	G	214	GLN
1	G	277	PRO
1	G	280	GLY
1	G	384	SER
1	H	214	GLN
1	H	277	PRO
1	H	280	GLY
1	H	441	ASN
1	H	486	ASN
1	A	383	ILE
1	B	338	SER
1	B	423	SER

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Mol	Chain	Res	Type
1	B	497	VAL
1	C	383	ILE
1	C	497	VAL
1	D	383	ILE
1	D	487	ALA
1	E	381	GLN
1	E	441	ASN
1	E	497	VAL
1	F	381	GLN
1	F	441	ASN
1	G	381	GLN
1	G	441	ASN
1	G	497	VAL
1	H	384	SER
1	H	497	VAL
1	A	338	SER
1	B	425	VAL
1	C	338	SER
1	C	425	VAL
1	C	485	GLY
1	D	338	SER
1	D	485	GLY
1	A	304	SER
1	B	304	SER
1	B	485	GLY
1	C	304	SER
1	D	304	SER
1	E	304	SER
1	F	304	SER
1	G	304	SER
1	H	304	SER
1	C	280	GLY
1	D	425	VAL
1	A	196	GLY
1	A	280	GLY
1	B	280	GLY
1	D	280	GLY

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	450/453 (99%)	408 (91%)	42 (9%)	8	29
1	B	450/453 (99%)	419 (93%)	31 (7%)	14	40
1	C	450/453 (99%)	410 (91%)	40 (9%)	9	31
1	D	450/453 (99%)	414 (92%)	36 (8%)	11	36
1	E	450/453 (99%)	412 (92%)	38 (8%)	10	34
1	F	450/453 (99%)	411 (91%)	39 (9%)	9	32
1	G	450/453 (99%)	407 (90%)	43 (10%)	8	28
1	H	450/453 (99%)	406 (90%)	44 (10%)	7	27
All	All	3600/3624 (99%)	3287 (91%)	313 (9%)	9	32

All (313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	70	ILE
1	A	105	GLN
1	A	142	LEU
1	A	154	VAL
1	A	183	LEU
1	A	192	PHE
1	A	195	GLU
1	A	198	LEU
1	A	212	THR
1	A	213	GLU
1	A	218	LYS
1	A	227	ILE
1	A	259	VAL
1	A	348	THR
1	A	350	THR
1	A	352	LEU
1	A	354	LYS
1	A	378	ASN
1	A	380	THR
1	A	381	GLN
1	A	382	THR
1	A	383	ILE

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Mol	Chain	Res	Type
1	A	386	SER
1	A	424	LYS
1	A	425	VAL
1	A	426	LYS
1	A	438	MET
1	A	440	VAL
1	A	447	SER
1	A	448	GLU
1	A	451	LEU
1	A	465	LEU
1	A	483	THR
1	A	484	THR
1	A	486	ASN
1	A	488	LEU
1	A	494	THR
1	A	497	VAL
1	A	498	ASP
1	A	500	LEU
1	A	508	VAL
1	B	5	THR
1	B	70	ILE
1	B	105	GLN
1	B	142	LEU
1	B	154	VAL
1	B	181	ASP
1	B	183	LEU
1	B	192	PHE
1	B	195	GLU
1	B	198	LEU
1	B	212	THR
1	B	213	GLU
1	B	218	LYS
1	B	227	ILE
1	B	259	VAL
1	B	350	THR
1	B	352	LEU
1	B	378	ASN
1	B	379	THR
1	B	381	GLN
1	B	382	THR
1	B	383	ILE
1	B	386	SER

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Mol	Chain	Res	Type
1	B	425	VAL
1	B	438	MET
1	B	440	VAL
1	B	465	LEU
1	B	483	THR
1	B	484	THR
1	B	494	THR
1	B	508	VAL
1	C	5	THR
1	C	22	ASP
1	C	70	ILE
1	C	105	GLN
1	C	142	LEU
1	C	154	VAL
1	C	181	ASP
1	C	184	LYS
1	C	192	PHE
1	C	195	GLU
1	C	198	LEU
1	C	212	THR
1	C	213	GLU
1	C	214	GLN
1	C	218	LYS
1	C	227	ILE
1	C	259	VAL
1	C	350	THR
1	C	352	LEU
1	C	356	ASN
1	C	378	ASN
1	C	380	THR
1	C	381	GLN
1	C	382	THR
1	C	383	ILE
1	C	386	SER
1	C	425	VAL
1	C	427	PHE
1	C	438	MET
1	C	440	VAL
1	C	446	LYS
1	C	447	SER
1	C	448	GLU
1	C	465	LEU

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Mol	Chain	Res	Type
1	C	483	THR
1	C	484	THR
1	C	494	THR
1	C	497	VAL
1	C	498	ASP
1	C	508	VAL
1	D	5	THR
1	D	22	ASP
1	D	70	ILE
1	D	105	GLN
1	D	142	LEU
1	D	154	VAL
1	D	180	SER
1	D	181	ASP
1	D	182	ASP
1	D	183	LEU
1	D	192	PHE
1	D	195	GLU
1	D	198	LEU
1	D	212	THR
1	D	218	LYS
1	D	227	ILE
1	D	259	VAL
1	D	350	THR
1	D	352	LEU
1	D	356	ASN
1	D	377	VAL
1	D	381	GLN
1	D	382	THR
1	D	384	SER
1	D	385	LYS
1	D	425	VAL
1	D	438	MET
1	D	440	VAL
1	D	448	GLU
1	D	463	ASN
1	D	465	LEU
1	D	483	THR
1	D	484	THR
1	D	494	THR
1	D	498	ASP
1	D	508	VAL

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Mol	Chain	Res	Type
1	E	5	THR
1	E	22	ASP
1	E	98	ASN
1	E	100	THR
1	E	141	VAL
1	E	142	LEU
1	E	147	THR
1	E	166	THR
1	E	181	ASP
1	E	183	LEU
1	E	194	ASN
1	E	198	LEU
1	E	200	TYR
1	E	214	GLN
1	E	225	ILE
1	E	278	THR
1	E	323	GLU
1	E	326	LEU
1	E	352	LEU
1	E	356	ASN
1	E	360	VAL
1	E	383	ILE
1	E	384	SER
1	E	385	LYS
1	E	396	LYS
1	E	398	LEU
1	E	426	LYS
1	E	428	VAL
1	E	429	LYS
1	E	430	GLU
1	E	437	ARG
1	E	448	GLU
1	E	465	LEU
1	E	483	THR
1	E	494	THR
1	E	497	VAL
1	E	498	ASP
1	E	500	LEU
1	F	4	GLU
1	F	5	THR
1	F	8	ARG
1	F	22	ASP

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Mol	Chain	Res	Type
1	F	98	ASN
1	F	99	ASP
1	F	141	VAL
1	F	142	LEU
1	F	147	THR
1	F	166	THR
1	F	181	ASP
1	F	183	LEU
1	F	194	ASN
1	F	198	LEU
1	F	200	TYR
1	F	214	GLN
1	F	225	ILE
1	F	254	ASP
1	F	278	THR
1	F	323	GLU
1	F	326	LEU
1	F	352	LEU
1	F	356	ASN
1	F	360	VAL
1	F	383	ILE
1	F	384	SER
1	F	385	LYS
1	F	396	LYS
1	F	398	LEU
1	F	426	LYS
1	F	429	LYS
1	F	430	GLU
1	F	431	ASN
1	F	448	GLU
1	F	465	LEU
1	F	483	THR
1	F	494	THR
1	F	497	VAL
1	F	498	ASP
1	G	4	GLU
1	G	5	THR
1	G	22	ASP
1	G	98	ASN
1	G	141	VAL
1	G	142	LEU
1	G	147	THR

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Mol	Chain	Res	Type
1	G	166	THR
1	G	181	ASP
1	G	183	LEU
1	G	194	ASN
1	G	198	LEU
1	G	200	TYR
1	G	214	GLN
1	G	225	ILE
1	G	253	PHE
1	G	278	THR
1	G	323	GLU
1	G	326	LEU
1	G	344	SER
1	G	348	THR
1	G	352	LEU
1	G	356	ASN
1	G	360	VAL
1	G	383	ILE
1	G	384	SER
1	G	387	VAL
1	G	398	LEU
1	G	400	ASP
1	G	424	LYS
1	G	425	VAL
1	G	426	LYS
1	G	428	VAL
1	G	429	LYS
1	G	430	GLU
1	G	431	ASN
1	G	448	GLU
1	G	465	LEU
1	G	483	THR
1	G	494	THR
1	G	497	VAL
1	G	498	ASP
1	G	500	LEU
1	H	4	GLU
1	H	5	THR
1	H	22	ASP
1	H	94	SER
1	H	97	PHE
1	H	98	ASN

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Mol	Chain	Res	Type
1	H	141	VAL
1	H	142	LEU
1	H	147	THR
1	H	166	THR
1	H	181	ASP
1	H	183	LEU
1	H	194	ASN
1	H	198	LEU
1	H	200	TYR
1	H	214	GLN
1	H	225	ILE
1	H	254	ASP
1	H	278	THR
1	H	323	GLU
1	H	326	LEU
1	H	327	ILE
1	H	345	ARG
1	H	352	LEU
1	H	356	ASN
1	H	360	VAL
1	H	383	ILE
1	H	384	SER
1	H	396	LYS
1	H	398	LEU
1	H	426	LYS
1	H	429	LYS
1	H	430	GLU
1	H	431	ASN
1	H	464	ILE
1	H	465	LEU
1	H	482	MET
1	H	483	THR
1	H	488	LEU
1	H	494	THR
1	H	495	THR
1	H	497	VAL
1	H	498	ASP
1	H	500	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	36	HIS
1	A	40	GLN
1	A	105	GLN
1	A	171	GLN
1	A	194	ASN
1	A	238	ASN
1	A	249	HIS
1	A	319	GLN
1	A	378	ASN
1	A	422	ASN
1	A	431	ASN
1	A	441	ASN
1	A	449	ASN
1	A	486	ASN
1	A	492	ASN
1	B	24	ASN
1	B	36	HIS
1	B	40	GLN
1	B	105	GLN
1	B	171	GLN
1	B	238	ASN
1	B	249	HIS
1	B	319	GLN
1	B	359	ASN
1	B	378	ASN
1	B	422	ASN
1	B	431	ASN
1	B	449	ASN
1	C	24	ASN
1	C	36	HIS
1	C	40	GLN
1	C	105	GLN
1	C	171	GLN
1	C	194	ASN
1	C	214	GLN
1	C	238	ASN
1	C	249	HIS
1	C	319	GLN
1	C	359	ASN
1	C	378	ASN
1	C	422	ASN
1	C	431	ASN

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Mol	Chain	Res	Type
1	C	462	GLN
1	D	24	ASN
1	D	36	HIS
1	D	40	GLN
1	D	105	GLN
1	D	171	GLN
1	D	194	ASN
1	D	238	ASN
1	D	249	HIS
1	D	319	GLN
1	D	359	ASN
1	D	422	ASN
1	D	431	ASN
1	D	441	ASN
1	E	24	ASN
1	E	36	HIS
1	E	40	GLN
1	E	64	ASN
1	E	98	ASN
1	E	105	GLN
1	E	148	GLN
1	E	161	GLN
1	E	171	GLN
1	E	194	ASN
1	E	228	ASN
1	E	249	HIS
1	E	270	GLN
1	E	364	ASN
1	E	422	ASN
1	E	441	ASN
1	E	507	GLN
1	F	24	ASN
1	F	36	HIS
1	F	40	GLN
1	F	64	ASN
1	F	105	GLN
1	F	145	ASN
1	F	148	GLN
1	F	171	GLN
1	F	194	ASN
1	F	249	HIS
1	F	356	ASN

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Mol	Chain	Res	Type
1	F	364	ASN
1	F	422	ASN
1	F	441	ASN
1	F	507	GLN
1	G	24	ASN
1	G	36	HIS
1	G	40	GLN
1	G	64	ASN
1	G	92	ASN
1	G	98	ASN
1	G	105	GLN
1	G	121	GLN
1	G	148	GLN
1	G	161	GLN
1	G	171	GLN
1	G	194	ASN
1	G	228	ASN
1	G	249	HIS
1	G	422	ASN
1	G	441	ASN
1	G	507	GLN
1	H	24	ASN
1	H	36	HIS
1	H	40	GLN
1	H	64	ASN
1	H	92	ASN
1	H	98	ASN
1	H	105	GLN
1	H	121	GLN
1	H	148	GLN
1	H	171	GLN
1	H	194	ASN
1	H	228	ASN
1	H	249	HIS
1	H	381	GLN
1	H	422	ASN
1	H	441	ASN
1	H	486	ASN
1	H	507	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	509/512 (99%)	0.29	20 (3%)	43	31	29, 37, 51, 70	0
1	B	509/512 (99%)	0.34	17 (3%)	49	36	29, 38, 49, 72	0
1	C	509/512 (99%)	0.53	29 (5%)	29	22	38, 50, 66, 79	0
1	D	509/512 (99%)	0.65	20 (3%)	43	31	37, 51, 68, 78	0
1	E	509/512 (99%)	0.58	35 (6%)	23	18	33, 47, 71, 114	0
1	F	509/512 (99%)	0.66	34 (6%)	24	19	31, 48, 75, 132	0
1	G	509/512 (99%)	0.95	60 (11%)	9	10	39, 59, 89, 130	0
1	H	509/512 (99%)	1.01	63 (12%)	8	9	40, 62, 93, 140	0
All	All	4072/4096 (99%)	0.63	278 (6%)	23	19	29, 48, 81, 140	0

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	382	THR	6.6
1	F	397	GLY	6.2
1	H	380	THR	5.7
1	H	228	ASN	5.0
1	G	100	THR	4.9
1	H	229	PRO	4.8
1	G	277	PRO	4.8
1	E	229	PRO	4.8
1	G	324	THR	4.8
1	A	382	THR	4.7
1	G	383	ILE	4.7
1	H	382	THR	4.7
1	F	324	THR	4.7
1	F	229	PRO	4.7
1	E	397	GLY	4.6
1	F	486	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	231	ALA	4.5
1	F	99	ASP	4.4
1	H	143	ALA	4.4
1	H	147	THR	4.4
1	G	148	GLN	4.4
1	H	486	ASN	4.3
1	H	146	SER	4.3
1	A	214	GLN	4.3
1	F	323	GLU	4.2
1	G	147	THR	4.2
1	F	147	THR	4.2
1	G	382	THR	4.2
1	G	339	ASN	4.2
1	G	229	PRO	4.2
1	H	170	SER	4.1
1	G	322	PRO	4.1
1	H	322	PRO	4.0
1	H	145	ASN	4.0
1	H	324	THR	4.0
1	B	255	ASN	4.0
1	F	383	ILE	4.0
1	H	385	LYS	4.0
1	A	349	ASN	4.0
1	D	277	PRO	3.9
1	F	321	ASN	3.9
1	C	486	ASN	3.9
1	G	146	SER	3.9
1	H	323	GLU	3.8
1	E	321	ASN	3.8
1	H	387	VAL	3.8
1	G	99	ASP	3.7
1	G	397	GLY	3.7
1	G	323	GLU	3.7
1	D	214	GLN	3.7
1	G	90	TYR	3.7
1	E	382	THR	3.6
1	G	381	GLN	3.6
1	F	146	SER	3.6
1	H	383	ILE	3.6
1	H	381	GLN	3.6
1	F	380	THR	3.6
1	H	117	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	378	ASN	3.5
1	D	486	ASN	3.4
1	E	487	ALA	3.4
1	F	228	ASN	3.4
1	C	448	GLU	3.4
1	G	170	SER	3.3
1	F	316	THR	3.3
1	F	320	ALA	3.3
1	C	397	GLY	3.3
1	H	397	GLY	3.3
1	G	321	ASN	3.2
1	G	258	ARG	3.2
1	F	319	GLN	3.2
1	F	230	GLY	3.2
1	G	486	ASN	3.2
1	E	316	THR	3.2
1	H	496	GLY	3.2
1	F	145	ASN	3.2
1	E	277	PRO	3.1
1	G	336	ASN	3.1
1	F	231	ALA	3.1
1	G	326	LEU	3.1
1	E	146	SER	3.1
1	F	170	SER	3.1
1	G	102	ASP	3.1
1	E	230	GLY	3.0
1	D	382	THR	3.0
1	E	214	GLN	3.0
1	C	382	THR	3.0
1	H	316	THR	3.0
1	A	496	GLY	3.0
1	G	340	ALA	3.0
1	E	144	ALA	2.9
1	F	143	ALA	2.9
1	H	137	GLN	2.9
1	D	38	TYR	2.9
1	C	99	ASP	2.9
1	D	32	ASP	2.9
1	H	142	LEU	2.9
1	H	431	ASN	2.9
1	G	384	SER	2.9
1	C	254	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	382	THR	2.9
1	C	339	ASN	2.9
1	H	277	PRO	2.9
1	E	339	ASN	2.9
1	G	88	VAL	2.9
1	F	322	PRO	2.8
1	D	193	ALA	2.8
1	H	386	SER	2.8
1	H	325	GLU	2.7
1	E	341	GLY	2.7
1	H	436	ASN	2.7
1	F	277	PRO	2.7
1	E	319	GLN	2.7
1	E	147	THR	2.7
1	G	36	HIS	2.7
1	C	277	PRO	2.7
1	D	423	SER	2.7
1	G	386	SER	2.7
1	H	339	ASN	2.7
1	H	347	ALA	2.6
1	F	341	GLY	2.6
1	G	496	GLY	2.6
1	B	277	PRO	2.6
1	G	129	GLY	2.6
1	B	5	THR	2.6
1	D	337	ILE	2.6
1	H	201	GLN	2.6
1	H	498	ASP	2.6
1	A	255	ASN	2.6
1	C	255	ASN	2.6
1	H	321	ASN	2.6
1	G	380	THR	2.6
1	G	214	GLN	2.6
1	H	489	GLY	2.6
1	F	182	ASP	2.5
1	D	380	THR	2.5
1	H	90	TYR	2.5
1	C	4	GLU	2.5
1	D	498	ASP	2.5
1	H	16	ASN	2.5
1	H	328	ASN	2.5
1	H	340	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	318	TYR	2.5
1	A	182	ASP	2.5
1	G	162	LYS	2.5
1	A	381	GLN	2.5
1	E	320	ALA	2.5
1	G	282	ALA	2.5
1	E	323	GLU	2.5
1	A	197	PHE	2.5
1	C	78	ASP	2.5
1	A	494	THR	2.5
1	C	191	ALA	2.4
1	H	313	SER	2.4
1	B	4	GLU	2.4
1	B	496	GLY	2.4
1	E	196	GLY	2.4
1	E	383	ILE	2.4
1	A	348	THR	2.4
1	H	99	ASP	2.4
1	H	182	ASP	2.4
1	E	90	TYR	2.4
1	E	231	ALA	2.4
1	C	384	SER	2.4
1	H	384	SER	2.4
1	H	183	LEU	2.4
1	A	277	PRO	2.4
1	G	316	THR	2.4
1	E	412	SER	2.4
1	C	485	GLY	2.4
1	G	230	GLY	2.4
1	H	230	GLY	2.4
1	B	90	TYR	2.4
1	C	385	LYS	2.4
1	C	341	GLY	2.3
1	C	91	ASN	2.3
1	D	426	LYS	2.3
1	G	145	ASN	2.3
1	G	319	GLN	2.3
1	H	350	THR	2.3
1	H	320	ALA	2.3
1	E	486	ASN	2.3
1	F	148	GLN	2.3
1	H	497	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	338	SER	2.3
1	C	383	ILE	2.3
1	D	386	SER	2.3
1	E	125	TYR	2.3
1	C	197	PHE	2.3
1	G	78	ASP	2.3
1	D	103	PRO	2.3
1	E	496	GLY	2.3
1	C	193	ALA	2.3
1	E	143	ALA	2.3
1	B	197	PHE	2.3
1	E	228	ASN	2.3
1	F	194	ASN	2.3
1	H	218	LYS	2.3
1	H	512	LYS	2.3
1	A	487	ALA	2.3
1	H	84	GLY	2.3
1	G	27	TRP	2.3
1	C	214	GLN	2.3
1	H	107	CYS	2.3
1	H	169	LYS	2.3
1	H	123	ILE	2.2
1	B	421	GLY	2.2
1	E	322	PRO	2.2
1	E	71	ALA	2.2
1	H	115	THR	2.2
1	H	219	SER	2.2
1	C	77	ASN	2.2
1	E	145	ASN	2.2
1	F	16	ASN	2.2
1	G	163	TRP	2.2
1	G	46	THR	2.2
1	G	278	THR	2.2
1	C	451	LEU	2.2
1	E	99	ASP	2.2
1	A	384	SER	2.2
1	D	307	SER	2.2
1	D	447	SER	2.2
1	B	214	GLN	2.2
1	C	337	ILE	2.2
1	A	385	LYS	2.2
1	G	385	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	396	LYS	2.2
1	D	197	PHE	2.2
1	G	115	THR	2.2
1	C	425	VAL	2.2
1	G	228	ASN	2.2
1	G	231	ALA	2.2
1	F	498	ASP	2.2
1	B	426	LYS	2.1
1	F	340	ALA	2.1
1	G	95	GLY	2.1
1	H	106	ARG	2.1
1	B	449	ASN	2.1
1	G	346	PHE	2.1
1	D	182	ASP	2.1
1	G	428	VAL	2.1
1	G	127	LEU	2.1
1	H	127	LEU	2.1
1	G	104	ARG	2.1
1	G	201	GLN	2.1
1	G	120	GLU	2.1
1	G	160	SER	2.1
1	E	91	ASN	2.1
1	G	337	ILE	2.1
1	A	195	GLU	2.1
1	C	499	ASN	2.1
1	A	361	ASP	2.1
1	E	385	LYS	2.1
1	H	355	ALA	2.1
1	H	487	ALA	2.1
1	B	341	GLY	2.1
1	D	496	GLY	2.1
1	A	497	VAL	2.1
1	B	75	LYS	2.1
1	H	98	ASN	2.1
1	C	380	THR	2.1
1	C	340	ALA	2.1
1	A	423	SER	2.0
1	G	190	SER	2.0
1	B	499	ASN	2.0
1	D	383	ILE	2.0
1	A	100	THR	2.0
1	F	318	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	4	GLU	2.0
1	F	497	VAL	2.0
1	B	383	ILE	2.0
1	B	384	SER	2.0
1	E	170	SER	2.0
1	A	380	THR	2.0
1	E	318	TYR	2.0
1	G	350	THR	2.0
1	H	153	LYS	2.0
1	G	110	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.