



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:03 PM UTC

PDB ID : 2WW0 / pdb_00002ww0
Title : Structure of the Family GH92 Inverting Mannosidase BT3990 from Bacteroides
thetaiotaomicron VPI-5482
Authors : Suits, M.D.L.; Thompson, A.; Zhu, Y.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2009-10-21
Resolution : 2.80 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

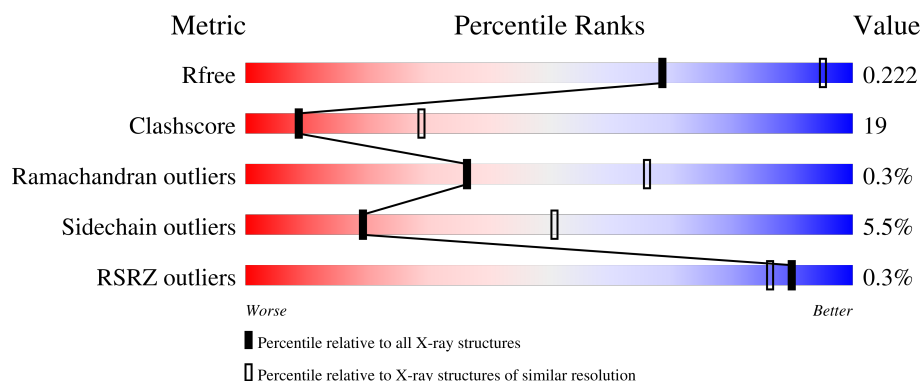
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

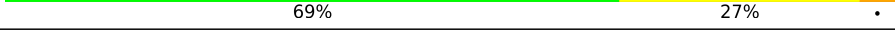
The reported resolution of this entry is 2.80 Å.

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.



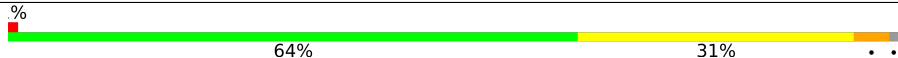
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	744	
1	B	744	
1	C	744	
1	D	744	
1	E	744	

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Mol	Chain	Length	Quality of chain
1	F	744	
1	G	744	
1	H	744	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	804	-	-	X	-
4	GOL	C	803	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 48426 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 PUTATIVE ALPHA-1,2-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	736	Total	C	N	O	S	0	3	0
			5977	3834	984	1125	34			
1	B	736	Total	C	N	O	S	0	5	0
			5997	3847	984	1131	35			
1	C	737	Total	C	N	O	S	0	2	0
			5979	3835	984	1126	34			
1	D	738	Total	C	N	O	S	0	2	0
			5984	3837	984	1129	34			
1	E	736	Total	C	N	O	S	0	2	0
			5956	3820	983	1120	33			
1	F	736	Total	C	N	O	S	0	1	0
			5954	3818	981	1121	34			
1	G	736	Total	C	N	O	S	0	0	0
			5932	3802	975	1123	32			
1	H	736	Total	C	N	O	S	0	0	0
			5899	3779	968	1120	32			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

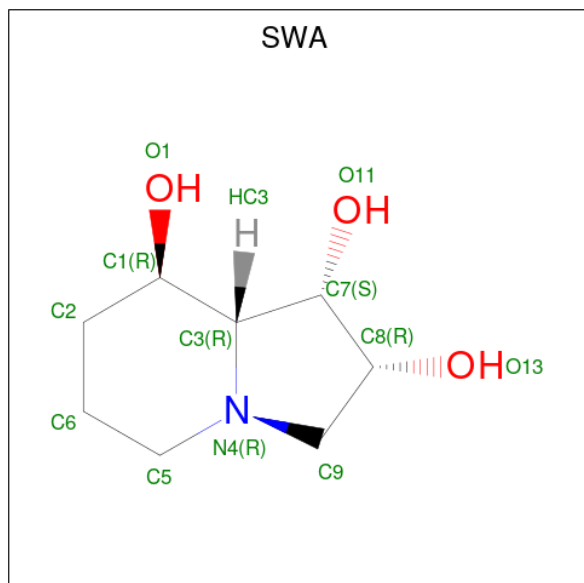
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ca	0	0
			1	1		
2	H	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 1S-8AB-OCTAHYDRO-INDOLIZIDINE-1A,2A,8B-TRIOLE (CCD ID: SWA) (formula: $C_8H_{15}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	8	1	3		
3	B	1	Total	C	N	O	0	0
			12	8	1	3		
3	C	1	Total	C	N	O	0	0
			12	8	1	3		
3	D	1	Total	C	N	O	0	0
			12	8	1	3		
3	E	1	Total	C	N	O	0	0
			12	8	1	3		
3	F	1	Total	C	N	O	0	0
			12	8	1	3		
3	G	1	Total	C	N	O	0	0
			12	8	1	3		
3	H	1	Total	C	N	O	0	0
			12	8	1	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

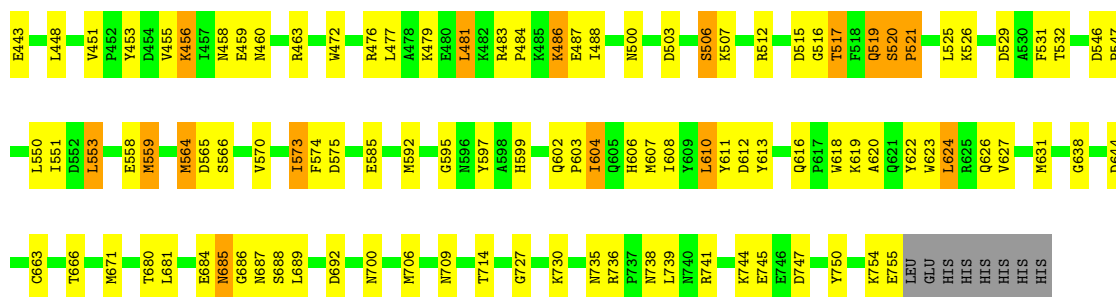
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

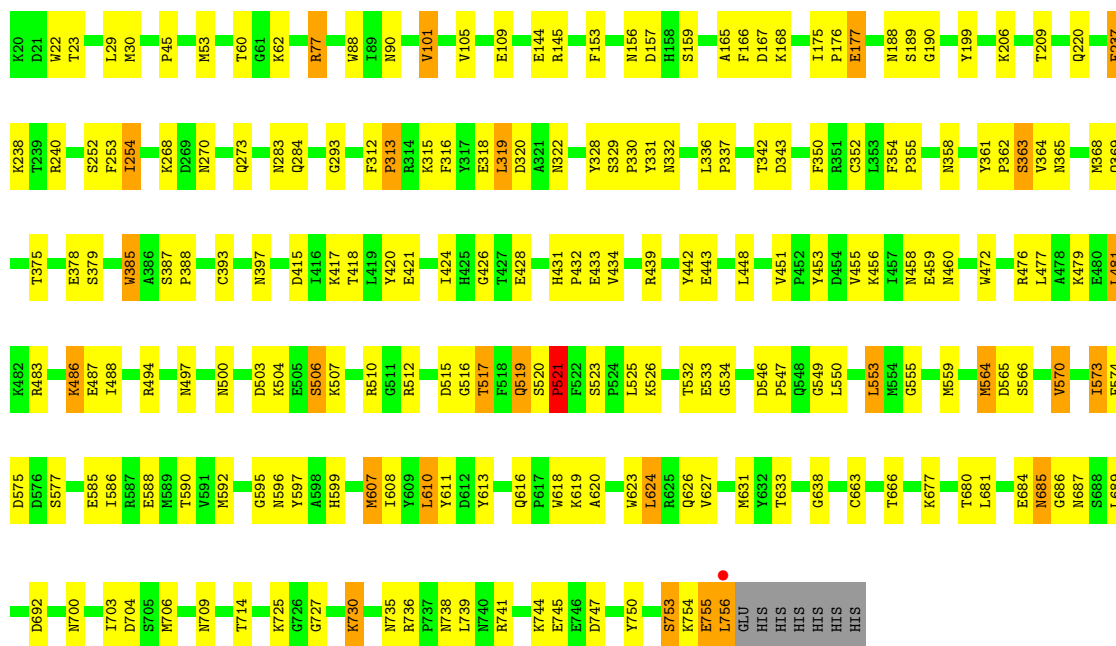
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	117	Total	O	0	0
			117	117		
5	B	105	Total	O	0	0
			105	105		
5	C	80	Total	O	0	0
			80	80		
5	D	110	Total	O	0	0
			110	110		
5	E	77	Total	O	0	0
			77	77		
5	F	42	Total	O	0	0
			42	42		
5	G	6	Total	O	0	0
			6	6		
5	H	5	Total	O	0	0
			5	5		



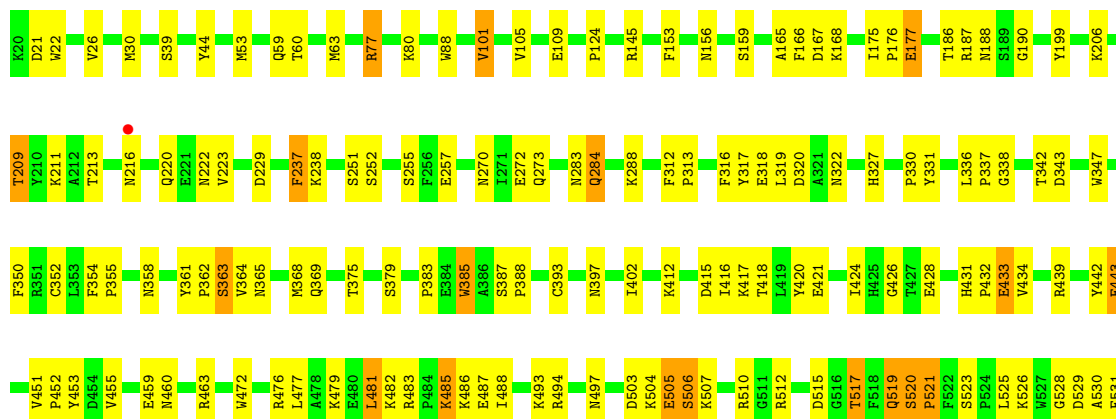
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

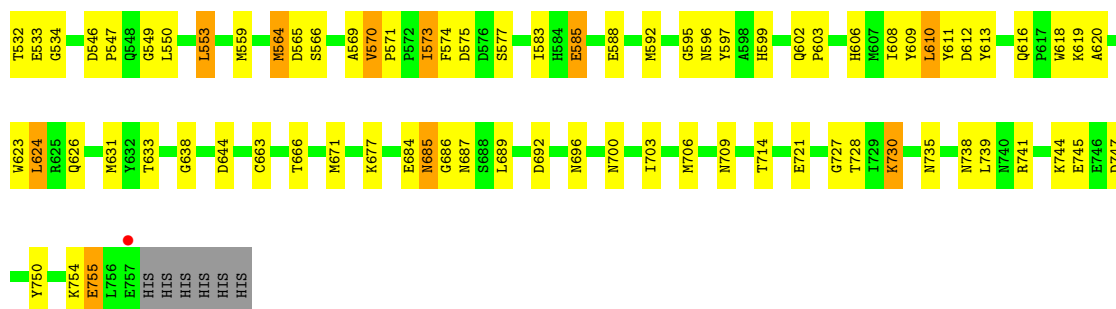
Chain C: 71% 24%



• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

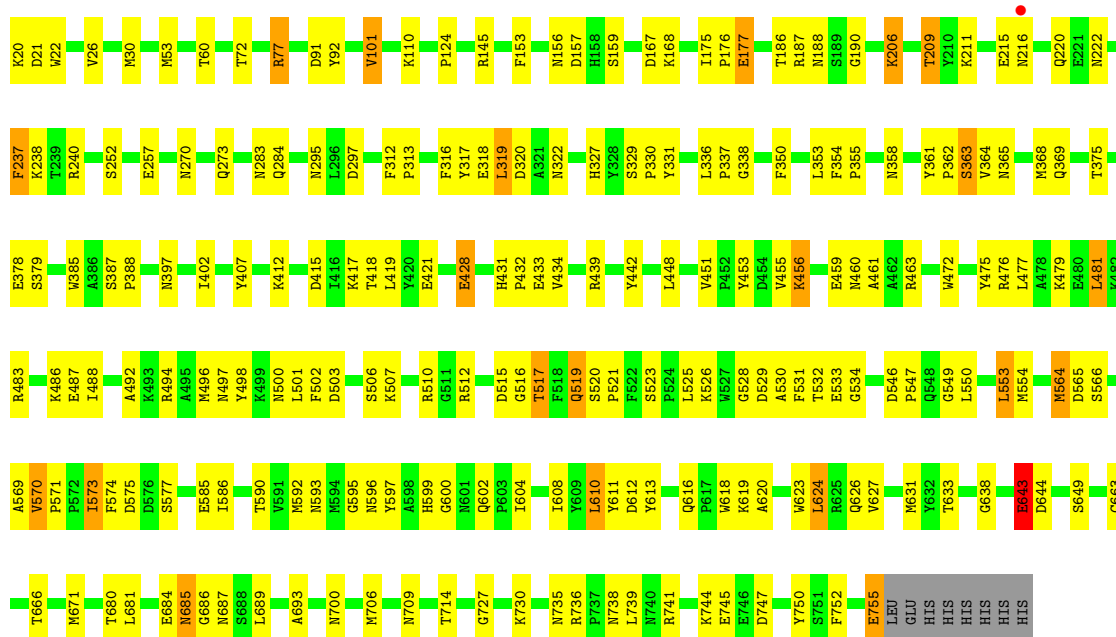
Chain D: 69% 27%





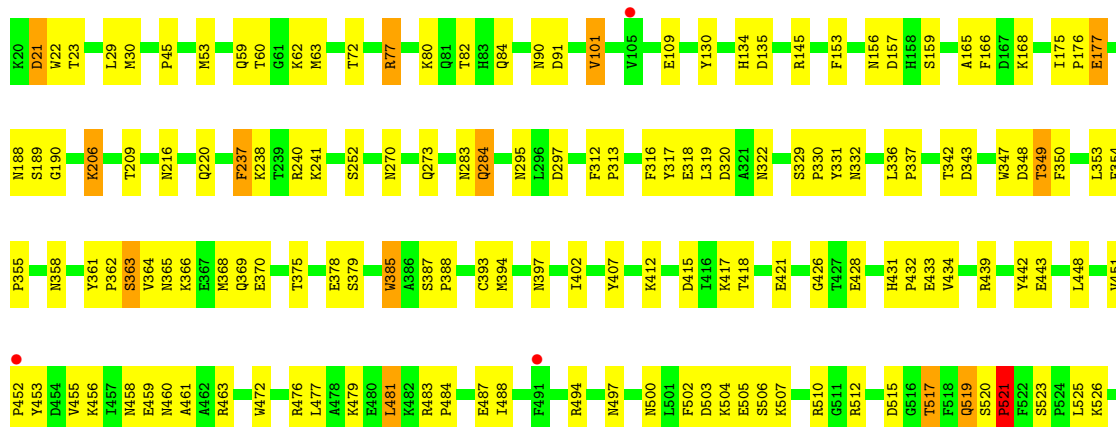
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

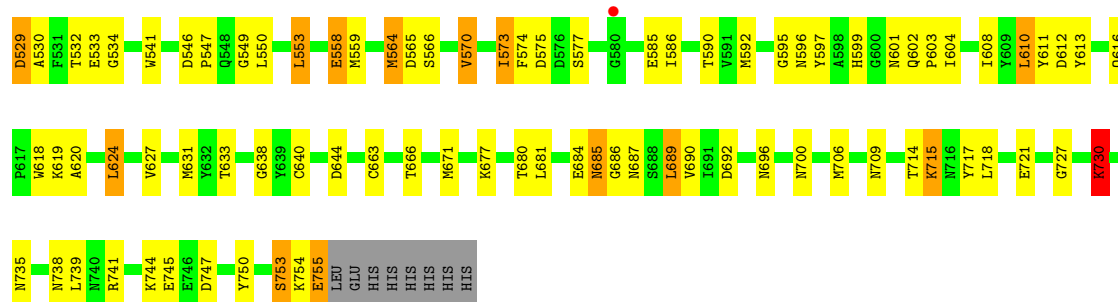
Chain E: 70% 26% ..



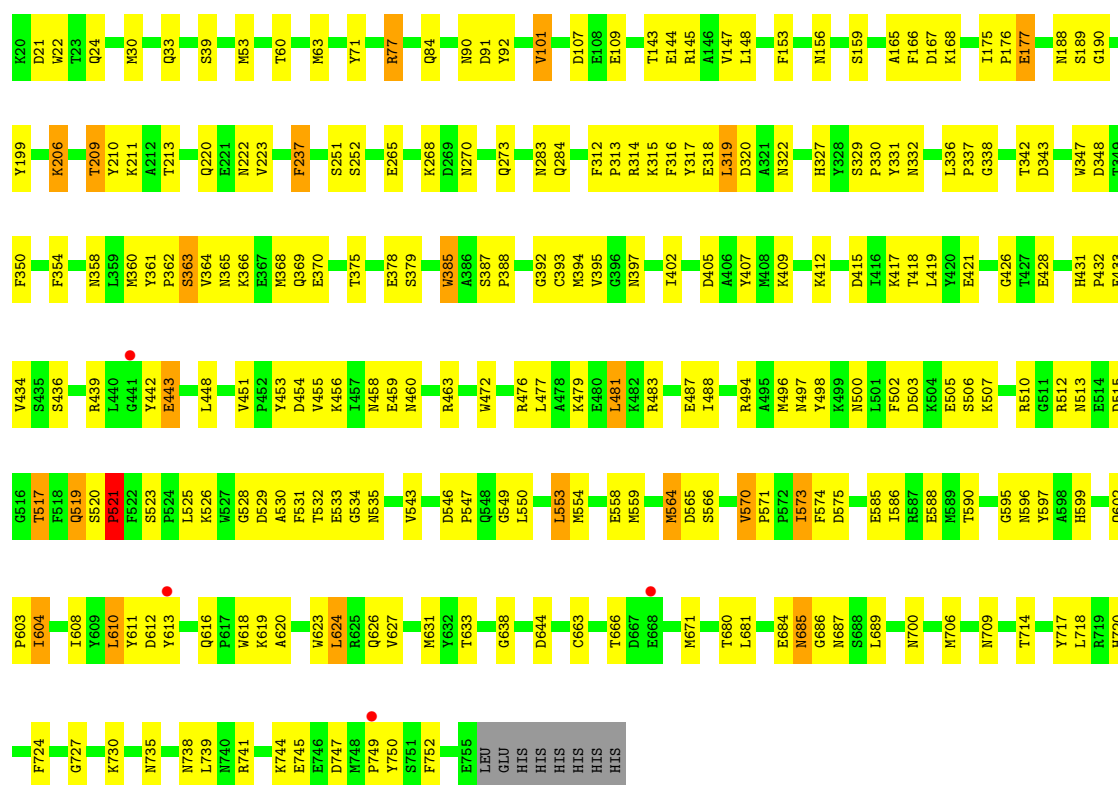
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain F: 68% 28% ..

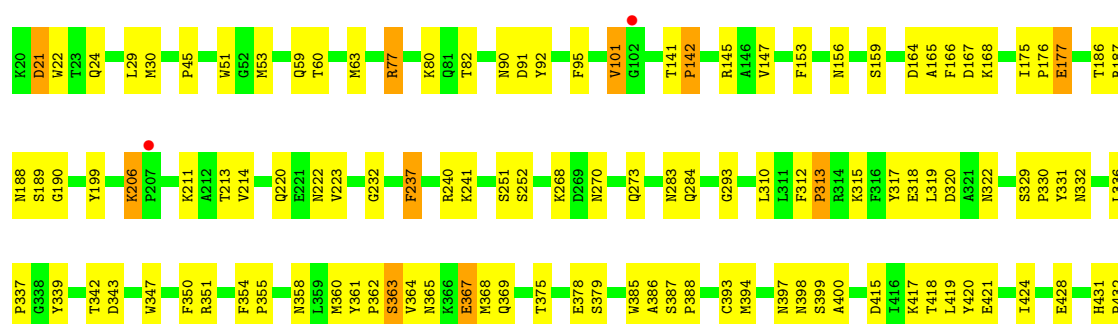


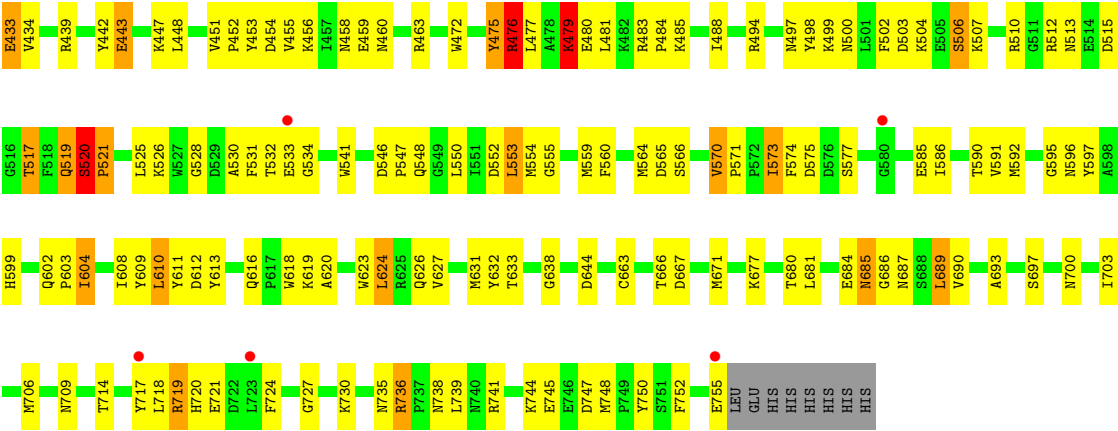


• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE



• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.81Å 151.96Å 218.62Å 90.00° 93.43° 90.00°	Depositor
Resolution (Å)	218.23 – 2.80 218.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (218.23-2.80) 97.9 (218.23-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.184 , 0.212 0.195 , 0.222	Depositor DCC
R_{free} test set	8504 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtrriage
Anisotropy	0.018	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	48426	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.64 % 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 7.7470e-04. 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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, SWA

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	0.69	0/6167	0.89	9/8365 (0.1%)
1	B	0.71	0/6193	0.89	3/8398 (0.0%)
1	C	0.67	0/6166	0.89	9/8365 (0.1%)
1	D	0.69	1/6171 (0.0%)	0.89	4/8373 (0.0%)
1	E	0.66	0/6143	0.89	7/8337 (0.1%)
1	F	0.60	0/6138	0.86	4/8330 (0.0%)
1	G	0.56	0/6113	0.85	3/8303 (0.0%)
1	H	0.58	1/6079 (0.0%)	0.87	9/8265 (0.1%)
All	All	0.65	2/49170 (0.0%)	0.88	48/66736 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
All	All	0	25

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	476	ARG	NE-CZ	6.24	1.40	1.33
1	D	416	ILE	CA-CB	-5.59	1.46	1.54

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	643	GLU	CB-CG-CD	8.16	126.47	112.60
1	H	638	GLY	N-CA-C	7.84	122.81	112.77
1	C	730	LYS	CB-CG-CD	7.22	127.91	111.30
1	D	638	GLY	N-CA-C	7.17	121.94	112.77
1	H	367	GLU	N-CA-C	-6.76	103.91	111.28
1	B	638	GLY	N-CA-C	6.71	122.36	113.37
1	E	643	GLU	CA-CB-CG	6.56	127.22	114.10
1	C	638	GLY	N-CA-C	6.40	120.96	112.77
1	A	638	GLY	N-CA-C	6.35	120.89	112.77
1	A	730	LYS	CB-CG-CD	6.28	125.74	111.30
1	D	730	LYS	CB-CG-CD	6.28	125.73	111.30
1	A	534	GLY	N-CA-C	-6.07	101.83	110.63
1	F	730	LYS	CB-CG-CD	6.03	125.16	111.30
1	E	209	THR	N-CA-C	-6.02	106.09	113.50
1	H	520	SER	C-N-CD	-5.91	107.60	120.60
1	H	313	PRO	N-CA-C	5.79	124.40	112.47
1	E	534	GLY	N-CA-C	-5.72	101.89	110.42
1	G	638	GLY	N-CA-C	5.72	121.04	113.37
1	F	534	GLY	N-CA-C	-5.67	102.47	110.75
1	E	638	GLY	N-CA-C	5.59	119.93	112.77
1	H	534	GLY	N-CA-C	-5.59	102.52	110.63
1	C	254	ILE	CB-CA-C	-5.53	107.01	111.71
1	F	638	GLY	N-CA-C	5.52	120.77	113.37
1	D	521	PRO	N-CA-C	5.47	123.75	112.47
1	A	521	PRO	N-CA-C	5.45	123.69	112.47
1	A	84	GLN	CA-C-N	5.40	126.59	119.84
1	A	84	GLN	C-N-CA	5.40	126.59	119.84
1	G	534	GLY	N-CA-C	-5.35	102.45	110.42
1	A	607	MET	N-CA-C	5.28	116.72	111.07
1	C	534	GLY	N-CA-C	-5.28	102.56	110.42
1	D	534	GLY	N-CA-C	-5.25	102.60	110.42
1	G	521	PRO	N-CA-C	5.25	123.28	112.47
1	C	254	ILE	N-CA-C	5.23	116.40	111.48
1	B	313	PRO	N-CA-C	5.22	123.22	112.47
1	H	521	PRO	N-CA-C	-5.21	98.56	112.10
1	H	479	LYS	N-CA-C	-5.20	105.51	111.07
1	B	143	THR	N-CA-C	-5.19	101.55	109.65
1	C	607	MET	N-CA-C	5.17	117.31	111.11
1	E	693	ALA	CA-C-N	5.15	125.44	119.47
1	E	693	ALA	C-N-CA	5.15	125.44	119.47
1	C	313	PRO	N-CA-C	5.13	123.03	112.47
1	A	451	VAL	CA-C-N	5.11	125.10	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	VAL	C-N-CA	5.11	125.10	119.89
1	F	521	PRO	N-CA-C	5.06	122.90	112.47
1	H	693	ALA	CA-C-N	5.03	125.31	119.47
1	H	693	ALA	C-N-CA	5.03	125.31	119.47
1	C	521	PRO	N-CA-C	5.01	122.80	112.47
1	C	755	GLU	N-CA-C	-5.01	106.39	113.20

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	PHE	Peptide
1	A	387	SER	Peptide
1	A	520	SER	Peptide
1	B	312	PHE	Peptide
1	B	387	SER	Peptide,Mainchain
1	B	520	SER	Peptide
1	C	312	PHE	Peptide
1	C	387	SER	Peptide
1	C	520	SER	Peptide
1	D	312	PHE	Peptide
1	D	387	SER	Peptide
1	D	520	SER	Peptide
1	E	312	PHE	Peptide
1	E	387	SER	Peptide
1	E	520	SER	Peptide
1	F	312	PHE	Peptide
1	F	387	SER	Peptide
1	F	520	SER	Peptide
1	G	312	PHE	Peptide
1	G	387	SER	Peptide
1	G	520	SER	Peptide
1	H	312	PHE	Peptide
1	H	387	SER	Peptide
1	H	520	SER	Mainchain

5.2 Too-close contacts [i](#)

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	5977	0	5654	192	0
1	B	5997	0	5677	212	0
1	C	5979	0	5652	177	0
1	D	5984	0	5647	202	0
1	E	5956	0	5614	187	0
1	F	5954	0	5610	231	0
1	G	5932	0	5554	248	0
1	H	5899	0	5483	294	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	13	2	0
3	B	12	0	14	2	0
3	C	12	0	14	4	0
3	D	12	0	14	5	0
3	E	12	0	14	1	0
3	F	12	0	13	5	0
3	G	12	0	13	5	0
3	H	12	0	12	5	0
4	A	30	0	40	3	0
4	B	18	0	24	6	0
4	C	18	0	24	6	0
4	D	18	0	24	4	0
4	E	12	0	16	0	0
4	F	6	0	8	0	0
5	A	117	0	0	6	0
5	B	105	0	0	11	0
5	C	80	0	0	2	0
5	D	110	0	0	14	0
5	E	77	0	0	2	0
5	F	42	0	0	8	0
5	G	6	0	0	0	0
5	H	5	0	0	0	0
All	All	48426	0	45134	1740	0

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

All (1740) 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:C:592[B]:MET:HE2	1:C:631:MET:CE	1.14	1.59
1:H:472:TRP:CE2	1:H:476:ARG:HD3	1.02	1.54
1:H:472:TRP:CE2	1:H:476:ARG:CD	1.92	1.52
1:B:592[B]:MET:CE	1:B:631:MET:HE1	1.05	1.51
1:H:472:TRP:CZ2	1:H:476:ARG:HD3	1.46	1.51
1:C:592[B]:MET:CE	1:C:631:MET:HE1	1.36	1.50
1:H:472:TRP:CZ2	1:H:476:ARG:CD	1.94	1.49
1:B:592[B]:MET:HE2	1:B:631:MET:CE	1.00	1.47
1:D:573:ILE:HD12	1:D:574:PHE:N	1.24	1.44
1:H:472:TRP:CD2	1:H:476:ARG:HD3	1.53	1.43
1:H:736:ARG:HH11	1:H:736:ARG:CB	1.31	1.42
1:H:472:TRP:CH2	1:H:476:ARG:NE	1.78	1.41
1:D:573:ILE:CD1	1:D:574:PHE:H	1.34	1.39
1:A:507:LYS:NZ	1:A:559:MET:HE2	1.34	1.38
1:H:483:ARG:O	1:H:488:ILE:CD1	1.71	1.37
1:F:730:LYS:HE2	5:F:2042:HOH:O	1.23	1.33
1:G:507:LYS:NZ	1:G:559:MET:HE1	1.41	1.33
1:G:550:LEU:HA	1:G:553:LEU:CD2	1.60	1.31
1:G:507:LYS:NZ	1:G:559:MET:CE	1.95	1.29
1:H:472:TRP:O	1:H:476:ARG:HG2	1.23	1.27
1:H:472:TRP:CZ2	1:H:476:ARG:NE	1.97	1.25
1:F:252:SER:OG	1:F:318:GLU:OE1	1.56	1.24
1:A:485:LYS:HE2	1:A:485:LYS:N	1.49	1.23
1:G:507:LYS:CE	1:G:559:MET:CE	2.15	1.23
1:C:573:ILE:HD12	1:C:574:PHE:N	1.52	1.22
1:G:706:MET:HE3	1:G:741:ARG:NH2	1.53	1.22
1:G:507:LYS:HE3	1:G:559:MET:CE	1.67	1.22
1:E:573:ILE:HD12	1:E:574:PHE:N	1.53	1.21
1:E:643:GLU:OE2	1:E:649:SER:OG	1.58	1.21
1:E:706:MET:HE3	1:E:741:ARG:NH2	1.54	1.21
1:G:363:SER:OG	1:G:684:GLU:CD	1.83	1.21
1:H:472:TRP:O	1:H:476:ARG:CG	1.88	1.20
1:A:485:LYS:CE	1:A:485:LYS:H	1.55	1.20
1:F:706:MET:HE3	1:F:741:ARG:NH2	1.55	1.19
1:H:375:THR:O	1:H:379:SER:OG	1.56	1.18
1:F:573:ILE:HD12	1:F:574:PHE:N	1.59	1.18
1:C:503:ASP:OD2	1:C:506:SER:OG	1.57	1.18
1:B:573:ILE:HD13	5:B:2078:HOH:O	1.42	1.17
1:G:573:ILE:HD12	1:G:574:PHE:N	1.56	1.17
1:H:736:ARG:HB3	1:H:736:ARG:NH1	1.57	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:397:ASN:ND2	1:G:439:ARG:HE	1.43	1.17
1:H:573:ILE:HD12	1:H:574:PHE:N	1.58	1.17
1:B:706:MET:HE3	1:B:741:ARG:NH2	1.60	1.17
1:C:706:MET:HE3	1:C:741:ARG:NH2	1.59	1.16
1:F:677:LYS:NZ	1:F:696:ASN:O	1.79	1.16
1:H:476:ARG:NH1	1:H:476:ARG:HB3	1.61	1.15
1:G:363:SER:OG	1:G:684:GLU:OE2	1.63	1.15
1:G:397:ASN:HD22	1:G:439:ARG:NE	1.42	1.15
1:H:592:MET:SD	1:H:631:MET:HE1	1.87	1.15
1:C:592[B]:MET:HE2	1:C:631:MET:HE3	1.29	1.14
1:H:483:ARG:C	1:H:488:ILE:HD11	1.73	1.13
1:H:706:MET:HE3	1:H:741:ARG:NH2	1.63	1.13
1:E:415:ASP:OD2	1:E:418:THR:OG1	1.67	1.12
1:A:706:MET:HE3	1:A:741:ARG:NH2	1.66	1.11
1:C:592[B]:MET:CE	1:C:631:MET:CE	2.08	1.10
1:F:546:ASP:CG	1:F:753:SER:OG	1.94	1.10
1:H:484:PRO:C	1:H:488:ILE:HD12	1.76	1.10
1:G:442:TYR:CZ	1:G:443:GLU:OE2	2.05	1.10
1:A:573:ILE:HD12	1:A:574:PHE:H	0.93	1.10
1:G:550:LEU:HA	1:G:553:LEU:HD21	1.30	1.09
1:H:211:LYS:NZ	1:H:222:ASN:OD1	1.84	1.08
1:G:442:TYR:CE2	1:G:443:GLU:OE2	2.04	1.08
1:H:82:THR:OG1	1:H:91:ASP:OD2	1.71	1.08
1:G:395:VAL:HG12	1:G:463:ARG:NH2	1.68	1.07
1:F:715:LYS:CE	1:F:717:TYR:OH	2.03	1.06
1:E:547:PRO:HG2	1:E:613:TYR:CE2	1.91	1.06
1:G:405:ASP:OD1	1:G:409:LYS:NZ	1.88	1.05
1:F:550:LEU:HA	1:F:553:LEU:HD12	1.35	1.05
3:B:801:SWA:HC91	5:B:2096:HOH:O	1.57	1.04
1:G:507:LYS:CE	1:G:559:MET:HE1	1.84	1.04
1:G:507:LYS:HE3	1:G:559:MET:HE3	1.40	1.04
1:H:483:ARG:O	1:H:488:ILE:HD11	0.86	1.03
1:F:157:ASP:OD1	1:F:238:LYS:HE3	1.58	1.03
1:F:715:LYS:NZ	1:F:717:TYR:CZ	2.25	1.03
1:F:546:ASP:OD1	1:F:753:SER:OG	1.74	1.03
1:A:573:ILE:HD12	1:A:574:PHE:N	1.72	1.02
1:F:547:PRO:HG2	1:F:613:TYR:CE2	1.93	1.02
1:C:573:ILE:CD1	1:C:574:PHE:H	1.73	1.02
1:F:546:ASP:OD2	1:F:753:SER:OG	1.75	1.02
1:F:715:LYS:HE2	1:F:717:TYR:CZ	1.95	1.02
1:H:481:LEU:N	1:H:481:LEU:HD23	1.72	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:472:TRP:HH2	1:H:476:ARG:HE	1.05	1.01
1:D:363:SER:OG	1:D:684:GLU:CD	2.03	1.01
1:D:363:SER:HG	1:D:684:GLU:CD	1.68	1.01
1:E:397:ASN:HD22	1:E:439:ARG:HE	1.04	1.01
1:F:715:LYS:HE2	1:F:717:TYR:OH	1.60	1.01
1:G:375:THR:O	1:G:379:SER:OG	1.79	1.01
1:B:252:SER:OG	1:B:318:GLU:OE1	1.76	1.00
1:G:167:ASP:OD1	1:G:168:LYS:HG2	1.62	1.00
1:G:550:LEU:CA	1:G:553:LEU:CD2	2.39	1.00
1:A:507:LYS:NZ	1:A:559:MET:CE	2.24	1.00
1:G:363:SER:OG	1:G:684:GLU:OE1	1.79	1.00
1:H:476:ARG:HB3	1:H:476:ARG:CZ	1.89	1.00
1:H:555:GLY:O	1:H:559:MET:CE	2.10	1.00
1:G:547:PRO:HG2	1:G:613:TYR:CE2	1.97	1.00
1:A:397:ASN:HD22	1:A:439:ARG:HE	1.00	1.00
1:H:736:ARG:CB	1:H:736:ARG:NH1	2.17	1.00
1:D:363:SER:OG	1:D:684:GLU:OE1	1.80	1.00
1:G:573:ILE:CD1	1:G:574:PHE:H	1.75	0.99
1:A:485:LYS:HE2	1:A:485:LYS:H	0.86	0.99
1:D:706:MET:HE3	1:D:741:ARG:NH2	1.77	0.99
1:H:592:MET:HE2	1:H:592:MET:HA	1.41	0.99
1:D:685:ASN:C	1:D:685:ASN:HD22	1.64	0.99
1:F:715:LYS:CE	1:F:717:TYR:CZ	2.46	0.99
1:E:573:ILE:CD1	1:E:574:PHE:H	1.75	0.99
1:H:573:ILE:HD12	1:H:574:PHE:H	0.82	0.98
1:H:736:ARG:HH11	1:H:736:ARG:HB3	0.83	0.98
1:H:252:SER:OG	1:H:318:GLU:OE1	1.80	0.98
1:D:507:LYS:NZ	1:D:559:MET:HE2	1.79	0.97
1:G:706:MET:HE3	1:G:741:ARG:HH22	1.14	0.97
1:F:503:ASP:OD2	1:F:506:SER:OG	1.79	0.97
1:E:706:MET:HE3	1:E:741:ARG:HH22	1.14	0.97
1:G:507:LYS:HZ1	1:G:559:MET:HE1	0.97	0.97
1:E:252:SER:OG	1:E:318:GLU:OE1	1.81	0.97
1:F:573:ILE:HD12	1:F:574:PHE:H	0.81	0.97
1:B:329:SER:OG	1:B:378:GLU:OE1	1.79	0.96
1:F:550:LEU:HA	1:F:553:LEU:CD1	1.95	0.96
1:H:472:TRP:CH2	1:H:476:ARG:CD	2.32	0.96
1:A:507:LYS:HZ1	1:A:559:MET:HE2	1.30	0.95
1:D:53:MET:HE2	1:D:145:ARG:HG2	1.49	0.95
1:G:442:TYR:CD2	1:G:443:GLU:OE2	2.18	0.95
1:F:592[B]:MET:CA	1:F:592[B]:MET:HE3	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:801:SWA:HC52	3:G:801:SWA:O13	1.62	0.95
1:G:507:LYS:NZ	1:G:559:MET:HE2	1.79	0.95
1:D:507:LYS:HZ2	1:D:559:MET:HE2	1.30	0.95
1:B:706:MET:HE3	1:B:741:ARG:HH22	1.31	0.95
1:B:157:ASP:OD1	1:B:238:LYS:HE3	1.68	0.94
1:H:503:ASP:OD2	1:H:506:SER:OG	1.86	0.94
1:F:546:ASP:CG	1:F:753:SER:HG	1.71	0.94
1:G:407:TYR:CE1	1:G:412:LYS:HE2	2.02	0.94
1:G:442:TYR:CE1	1:G:443:GLU:OE2	2.21	0.94
1:H:685:ASN:C	1:H:685:ASN:HD22	1.75	0.94
1:C:546:ASP:OD1	1:C:753:SER:OG	1.85	0.94
1:D:684:GLU:OE2	4:D:804:GOL:O3	1.85	0.94
1:F:706:MET:HE3	1:F:741:ARG:HH22	1.20	0.94
1:A:550:LEU:HA	1:A:553:LEU:HD12	1.50	0.93
1:C:157:ASP:OD1	1:C:238:LYS:HE3	1.69	0.92
1:G:507:LYS:HZ2	1:G:559:MET:HE2	1.30	0.92
1:F:592[B]:MET:SD	1:F:631:MET:HE1	2.09	0.92
1:D:685:ASN:HD22	1:D:686:GLY:N	1.66	0.92
1:H:706:MET:HE3	1:H:741:ARG:HH22	1.23	0.92
1:G:685:ASN:C	1:G:685:ASN:HD22	1.76	0.92
1:F:685:ASN:HD22	1:F:685:ASN:C	1.77	0.91
1:B:363:SER:OG	1:B:684:GLU:OE2	1.88	0.91
1:F:397:ASN:ND2	1:F:439:ARG:HE	1.68	0.91
1:E:397:ASN:ND2	1:E:439:ARG:HE	1.68	0.91
1:E:550:LEU:HA	1:E:553:LEU:HD12	1.50	0.91
1:A:685:ASN:HD22	1:A:685:ASN:C	1.76	0.91
1:F:82:THR:OG1	1:F:91:ASP:OD2	1.88	0.91
1:C:550:LEU:HA	1:C:553:LEU:HD12	1.53	0.91
1:F:397:ASN:HD22	1:F:439:ARG:NE	1.70	0.90
1:H:329:SER:OG	1:H:378:GLU:OE1	1.87	0.90
1:C:706:MET:HE3	1:C:741:ARG:HH22	1.31	0.90
1:H:573:ILE:CD1	1:H:574:PHE:H	1.79	0.90
1:H:347:TRP:CZ3	3:H:801:SWA:HC7	2.07	0.90
1:H:608:ILE:HG21	1:H:624:LEU:HD13	1.54	0.90
1:A:53:MET:HE2	1:A:145:ARG:HG2	1.54	0.89
1:A:252:SER:OG	1:A:318:GLU:OE1	1.90	0.89
1:F:730:LYS:CE	5:F:2042:HOH:O	1.94	0.89
1:F:592[B]:MET:HE3	1:F:592[B]:MET:HA	1.53	0.89
1:C:254:ILE:O	4:C:803:GOL:H31	1.73	0.89
1:H:472:TRP:CD2	1:H:476:ARG:CD	2.38	0.89
1:H:547:PRO:HG2	1:H:613:TYR:CE2	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:SER:OG	1:E:684:GLU:CD	2.16	0.89
1:F:375:THR:O	1:F:379:SER:OG	1.90	0.89
1:F:397:ASN:HD22	1:F:439:ARG:HE	0.89	0.88
1:H:339:TYR:CD1	1:H:367:GLU:HG2	2.08	0.88
1:B:529:ASP:HB3	5:B:2075:HOH:O	1.73	0.88
1:F:592[B]:MET:HE2	1:F:631:MET:HE1	1.56	0.88
1:B:550:LEU:HA	1:B:553:LEU:HD12	1.56	0.88
1:G:685:ASN:ND2	1:G:687:ASN:H	1.70	0.88
1:F:685:ASN:ND2	1:F:687:ASN:H	1.72	0.88
1:H:555:GLY:O	1:H:559:MET:HE3	1.71	0.88
1:G:53:MET:HE2	1:G:145:ARG:HG2	1.54	0.88
1:C:592[B]:MET:SD	1:C:631:MET:HE1	2.14	0.88
1:F:573:ILE:CD1	1:F:574:PHE:H	1.78	0.88
1:F:329:SER:OG	1:F:378:GLU:OE1	1.92	0.87
1:A:375:THR:O	1:A:379:SER:OG	1.91	0.87
1:D:550:LEU:HA	1:D:553:LEU:HD12	1.57	0.87
1:D:685:ASN:ND2	1:D:687:ASN:H	1.71	0.87
1:G:454:ASP:OD2	1:G:513:ASN:HB3	1.73	0.87
1:H:472:TRP:CH2	1:H:476:ARG:HD3	2.03	0.87
1:B:363:SER:OG	1:B:684:GLU:CD	2.17	0.87
1:H:484:PRO:O	1:H:488:ILE:HD12	1.73	0.87
1:A:431:HIS:HD2	1:A:433:GLU:H	1.23	0.87
1:G:366:LYS:NZ	1:G:370:GLU:OE2	2.06	0.87
1:F:715:LYS:NZ	1:F:717:TYR:CE2	2.40	0.86
1:C:397:ASN:HD22	1:C:439:ARG:HE	1.16	0.86
1:B:486:LYS:H	1:B:486:LYS:HD3	1.39	0.86
1:G:407:TYR:CE2	1:G:412:LYS:HD3	2.11	0.86
1:A:706:MET:HE3	1:A:741:ARG:HH22	1.34	0.86
1:C:375:THR:O	1:C:379:SER:OG	1.94	0.86
1:D:272:GLU:HG3	4:D:802:GOL:H31	1.58	0.86
1:E:363:SER:OG	1:E:684:GLU:OE2	1.93	0.86
1:A:507:LYS:HZ2	1:A:559:MET:HE2	1.03	0.85
1:D:706:MET:HE3	1:D:741:ARG:HH22	1.39	0.85
1:H:685:ASN:ND2	1:H:687:ASN:H	1.72	0.85
1:E:685:ASN:C	1:E:685:ASN:HD22	1.81	0.85
1:A:685:ASN:ND2	1:A:687:ASN:H	1.73	0.85
1:D:431:HIS:HD2	1:D:433:GLU:H	1.24	0.85
1:D:566:SER:O	1:D:570:VAL:HG13	1.77	0.85
1:D:573:ILE:CD1	1:D:574:PHE:N	2.07	0.85
1:C:685:ASN:HD22	1:C:685:ASN:C	1.82	0.84
1:B:547:PRO:HG2	1:B:613:TYR:CE2	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:685:ASN:ND2	1:E:687:ASN:H	1.76	0.84
1:E:157:ASP:HA	1:E:238:LYS:HG2	1.58	0.84
1:D:507:LYS:NZ	1:D:559:MET:CE	2.40	0.84
1:B:375:THR:O	1:B:379:SER:OG	1.94	0.83
1:B:592[B]:MET:CE	1:B:631:MET:CE	1.92	0.83
1:D:363:SER:OG	1:D:684:GLU:OE2	1.94	0.83
1:E:608:ILE:HG21	1:E:624:LEU:HD13	1.59	0.83
1:A:298:GLN:HE22	4:A:803:GOL:H2	1.41	0.83
1:E:415:ASP:CG	1:E:418:THR:OG1	2.22	0.83
1:C:588:GLU:O	1:C:592[A]:MET:HE3	1.78	0.83
1:A:397:ASN:ND2	1:A:439:ARG:HE	1.77	0.83
1:B:685:ASN:C	1:B:685:ASN:HD22	1.86	0.83
1:H:347:TRP:HZ3	3:H:801:SWA:HC7	1.44	0.83
1:F:592[B]:MET:CE	1:F:631:MET:HE1	2.08	0.83
1:D:573:ILE:HD12	1:D:574:PHE:H	0.66	0.83
1:G:507:LYS:HZ2	1:G:559:MET:CE	1.83	0.83
1:G:252:SER:OG	1:G:318:GLU:OE1	1.97	0.82
1:A:685:ASN:HD22	1:A:686:GLY:N	1.76	0.82
1:H:397:ASN:HD22	1:H:439:ARG:HE	1.27	0.82
1:B:608:ILE:HG21	1:B:624:LEU:HD13	1.61	0.82
1:C:685:ASN:ND2	1:C:687:ASN:H	1.77	0.82
1:F:366:LYS:NZ	1:F:370:GLU:OE2	2.13	0.82
1:G:167:ASP:O	1:G:168:LYS:HB2	1.79	0.82
1:H:339:TYR:CE1	1:H:367:GLU:HG2	2.15	0.82
1:F:507:LYS:HE3	1:F:559:MET:HE2	1.61	0.81
1:B:573:ILE:HD12	1:B:574:PHE:H	1.44	0.81
1:D:608:ILE:HG21	1:D:624:LEU:HD13	1.62	0.81
1:H:564:MET:HE1	1:H:610:LEU:HB2	1.62	0.81
1:E:397:ASN:HD22	1:E:439:ARG:NE	1.79	0.81
1:B:685:ASN:ND2	1:B:687:ASN:H	1.78	0.81
1:B:431:HIS:HD2	1:B:433:GLU:H	1.26	0.81
1:G:211:LYS:NZ	1:G:222:ASN:OD1	2.14	0.81
1:F:510:ARG:NH2	1:F:519:GLN:O	2.12	0.81
1:H:331:TYR:CZ	1:H:375:THR:HG23	2.16	0.81
1:H:472:TRP:CE3	1:H:476:ARG:HD3	2.13	0.80
1:G:685:ASN:HD22	1:G:686:GLY:N	1.78	0.80
1:G:395:VAL:HG12	1:G:463:ARG:CZ	2.11	0.80
1:E:573:ILE:HD12	1:E:574:PHE:H	0.79	0.80
1:F:216:ASN:HB2	5:F:2021:HOH:O	1.81	0.80
1:H:472:TRP:CE3	1:H:476:ARG:HG3	2.16	0.80
1:E:566:SER:O	1:E:570:VAL:HG13	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:503:ASP:OD2	1:G:506:SER:OG	1.99	0.80
1:A:547:PRO:HG2	1:A:613:TYR:CE2	2.17	0.79
1:F:550:LEU:CA	1:F:553:LEU:HD12	2.13	0.79
1:F:608:ILE:HG21	1:F:624:LEU:HD13	1.64	0.79
1:G:608:ILE:HG21	1:G:624:LEU:HD13	1.65	0.79
1:D:22:TRP:H	1:D:283:ASN:ND2	1.80	0.79
1:F:558:GLU:HB3	5:F:2038:HOH:O	1.80	0.79
1:G:442:TYR:CD1	1:G:443:GLU:OE2	2.34	0.79
1:C:547:PRO:HG2	1:C:613:TYR:CE2	2.18	0.79
1:G:442:TYR:CG	1:G:443:GLU:OE2	2.35	0.79
1:H:566:SER:O	1:H:570:VAL:HG13	1.83	0.79
1:B:486:LYS:H	1:B:486:LYS:CD	1.95	0.79
1:C:431:HIS:HD2	1:C:433:GLU:H	1.30	0.79
1:G:407:TYR:CZ	1:G:412:LYS:HD3	2.18	0.79
1:H:685:ASN:HD22	1:H:686:GLY:N	1.80	0.79
1:E:550:LEU:HA	1:E:553:LEU:CD1	2.12	0.79
1:G:498:TYR:OH	1:G:546:ASP:OD2	2.01	0.79
1:G:525:LEU:HD13	1:G:573:ILE:HG23	1.64	0.79
1:A:675:LEU:O	4:A:803:GOL:H11	1.83	0.79
1:H:442:TYR:CZ	1:H:443:GLU:OE2	2.36	0.79
1:H:735:ASN:OD1	1:H:736:ARG:HD2	1.81	0.79
1:C:608:ILE:HG21	1:C:624:LEU:HD13	1.65	0.78
1:G:507:LYS:CE	1:G:559:MET:HE2	2.09	0.78
1:G:573:ILE:HD12	1:G:574:PHE:H	0.78	0.78
1:F:348:ASP:OD1	3:F:801:SWA:O1	2.00	0.78
1:F:592[B]:MET:HA	1:F:592[B]:MET:CE	2.12	0.78
1:A:397:ASN:HD22	1:A:439:ARG:NE	1.81	0.78
1:A:507:LYS:HZ1	1:A:559:MET:CE	1.88	0.78
1:F:685:ASN:HD22	1:F:686:GLY:N	1.80	0.78
1:H:442:TYR:CE1	1:H:443:GLU:OE2	2.37	0.78
1:G:415:ASP:OD2	1:G:418:THR:OG1	2.02	0.78
1:B:315:LYS:NZ	4:B:804:GOL:H32	1.98	0.78
1:D:22:TRP:H	1:D:283:ASN:HD21	1.32	0.78
1:F:442:TYR:CZ	1:F:443:GLU:OE2	2.37	0.78
1:G:549:GLY:O	1:G:553:LEU:CD2	2.31	0.78
1:A:564:MET:HE1	1:A:610:LEU:HB2	1.65	0.78
1:G:405:ASP:CG	1:G:409:LYS:HZ1	1.92	0.77
1:E:525:LEU:HD13	1:E:573:ILE:HG23	1.66	0.77
1:G:550:LEU:HA	1:G:553:LEU:HD23	1.62	0.77
1:B:397:ASN:HD22	1:B:439:ARG:HE	1.32	0.77
1:F:252:SER:OG	1:F:318:GLU:CD	2.27	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:ARG:NH2	1:H:317:TYR:O	2.13	0.77
1:H:481:LEU:N	1:H:481:LEU:CD2	2.48	0.77
1:C:397:ASN:ND2	1:C:439:ARG:HE	1.83	0.77
1:H:476:ARG:NH1	1:H:476:ARG:CB	2.47	0.77
1:G:431:HIS:HD2	1:G:433:GLU:H	1.32	0.77
1:G:566:SER:O	1:G:570:VAL:HG13	1.85	0.77
1:F:331:TYR:CZ	1:F:375:THR:HG23	2.20	0.77
1:B:442:TYR:CE1	1:B:443:GLU:OE2	2.38	0.77
1:D:397:ASN:HD22	1:D:439:ARG:HE	1.33	0.77
1:H:515:ASP:OD1	1:H:517:THR:OG1	2.03	0.77
1:B:486:LYS:HD3	1:B:486:LYS:N	2.00	0.76
1:G:528:GLY:HA2	1:G:531:PHE:O	1.85	0.76
1:G:564:MET:HE1	1:G:610:LEU:HB2	1.66	0.76
1:F:358:ASN:ND2	1:F:365:ASN:HD22	1.84	0.76
1:H:744:LYS:HB2	1:H:747:ASP:OD2	1.85	0.76
1:B:109:GLU:HB2	1:E:110:LYS:NZ	2.01	0.76
1:E:506:SER:O	1:E:507:LYS:HB2	1.86	0.76
1:E:706:MET:CE	1:E:741:ARG:HH22	1.97	0.76
1:H:503:ASP:CG	1:H:506:SER:OG	2.29	0.76
1:C:573:ILE:HD12	1:C:574:PHE:H	0.76	0.76
1:E:363:SER:OG	1:E:684:GLU:OE1	2.04	0.75
3:G:801:SWA:O13	3:G:801:SWA:C5	2.34	0.75
1:A:507:LYS:CE	1:A:559:MET:HE2	2.16	0.75
1:H:476:ARG:HB3	1:H:476:ARG:HH11	1.50	0.75
1:G:706:MET:CE	1:G:741:ARG:HH22	1.96	0.75
1:F:525:LEU:HD13	1:F:573:ILE:HG23	1.69	0.75
1:H:472:TRP:O	1:H:476:ARG:HG3	1.84	0.75
1:B:107:ASP:OD2	1:E:110:LYS:HE2	1.86	0.74
1:B:564:MET:HE1	1:B:610:LEU:HB2	1.69	0.74
1:F:442:TYR:CE1	1:F:443:GLU:OE2	2.39	0.74
1:G:680:THR:C	1:G:681:LEU:HD23	2.12	0.74
1:H:442:TYR:CD1	1:H:443:GLU:OE2	2.40	0.74
1:H:592:MET:HE2	1:H:592:MET:CA	2.17	0.74
1:F:503:ASP:CG	1:F:506:SER:OG	2.29	0.74
1:H:608:ILE:CG2	1:H:624:LEU:HD13	2.16	0.74
1:D:564:MET:HE1	1:D:610:LEU:HB2	1.69	0.74
1:G:553:LEU:HD22	1:G:553:LEU:H	1.52	0.74
1:G:744:LYS:HB2	1:G:747:ASP:OD2	1.87	0.74
1:H:472:TRP:CZ3	1:H:476:ARG:CD	2.70	0.74
1:E:215:GLU:O	1:E:216[B]:ASN:OD1	2.05	0.74
1:C:22:TRP:H	1:C:283:ASN:ND2	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:431:HIS:HD2	1:F:433:GLU:H	1.33	0.74
1:F:592[B]:MET:HE2	1:F:631:MET:CE	2.18	0.74
1:H:442:TYR:CE2	1:H:443:GLU:OE2	2.41	0.74
1:A:363:SER:HG	1:A:684:GLU:CD	1.96	0.74
1:F:459:GLU:HG2	1:F:532:THR:HG22	1.70	0.74
1:D:547:PRO:HG2	1:D:613:TYR:CE2	2.22	0.74
1:H:315:LYS:HE2	1:H:317:TYR:OH	1.87	0.74
1:C:503:ASP:CG	1:C:506:SER:OG	2.30	0.73
1:E:643:GLU:CD	1:E:649:SER:HG	1.90	0.73
1:B:22:TRP:H	1:B:283:ASN:ND2	1.84	0.73
1:F:503:ASP:CG	1:F:506:SER:HG	1.93	0.73
1:F:715:LYS:HE2	1:F:717:TYR:CE1	2.22	0.73
1:A:211:LYS:NZ	1:A:222:ASN:OD1	2.21	0.73
1:A:685:ASN:C	1:A:685:ASN:ND2	2.45	0.73
1:A:550:LEU:HA	1:A:553:LEU:CD1	2.16	0.73
1:B:550:LEU:HA	1:B:553:LEU:CD1	2.18	0.73
1:C:252:SER:OG	1:C:318:GLU:OE1	2.04	0.73
1:C:550:LEU:HA	1:C:553:LEU:CD1	2.17	0.73
1:H:685:ASN:C	1:H:685:ASN:ND2	2.45	0.73
1:C:442:TYR:CE1	1:C:443:GLU:OE2	2.41	0.73
1:B:358:ASN:ND2	1:B:365:ASN:HD22	1.87	0.73
1:B:515:ASP:C	1:B:515:ASP:OD1	2.32	0.73
1:B:566:SER:O	1:B:570:VAL:HG13	1.88	0.73
1:D:188:ASN:HD22	1:D:190:GLY:H	1.36	0.73
1:E:407:TYR:CE2	1:E:412:LYS:HG2	2.24	0.72
1:D:685:ASN:C	1:D:685:ASN:ND2	2.35	0.72
1:C:685:ASN:HD22	1:C:686:GLY:N	1.88	0.72
1:H:331:TYR:CE2	1:H:375:THR:HG23	2.24	0.72
1:H:442:TYR:CD2	1:H:443:GLU:OE2	2.43	0.72
1:B:442:TYR:CZ	1:B:443:GLU:OE2	2.42	0.72
1:D:608:ILE:CG2	1:D:624:LEU:HD13	2.19	0.72
1:E:515:ASP:C	1:E:515:ASP:OD1	2.32	0.72
1:H:431:HIS:HD2	1:H:433:GLU:H	1.35	0.72
1:H:680:THR:C	1:H:681:LEU:HD23	2.15	0.72
1:F:706:MET:CE	1:F:741:ARG:HH22	1.99	0.72
1:H:484:PRO:C	1:H:488:ILE:CD1	2.61	0.72
1:H:592:MET:SD	1:H:631:MET:CE	2.73	0.72
1:F:755:GLU:C	1:F:755:GLU:OE1	2.33	0.72
1:H:736:ARG:HH11	1:H:736:ARG:CG	2.02	0.72
1:A:525:LEU:HD13	1:A:573:ILE:HG23	1.72	0.71
1:F:744:LYS:HB2	1:F:747:ASP:OD2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:LYS:HD2	1:H:237:PHE:CD1	2.25	0.71
1:H:415:ASP:OD2	1:H:418:THR:OG1	2.07	0.71
1:E:608:ILE:CG2	1:E:624:LEU:HD13	2.20	0.71
1:A:216:ASN:HB3	5:A:2035:HOH:O	1.90	0.71
1:E:431:HIS:HD2	1:E:433:GLU:H	1.38	0.71
1:G:331:TYR:CZ	1:G:375:THR:HG23	2.26	0.71
1:H:736:ARG:HH11	1:H:736:ARG:HB2	1.51	0.71
1:B:188:ASN:HD22	1:B:190:GLY:H	1.37	0.71
1:G:415:ASP:CG	1:G:418:THR:OG1	2.34	0.71
1:G:483:ARG:O	1:G:488:ILE:HD11	1.91	0.71
1:H:350:PHE:C	1:H:350:PHE:CD2	2.69	0.71
1:E:685:ASN:HD22	1:E:686:GLY:N	1.89	0.70
1:B:685:ASN:HD22	1:B:686:GLY:N	1.89	0.70
1:F:21:ASP:OD1	1:F:21:ASP:C	2.34	0.70
1:C:442:TYR:CZ	1:C:443:GLU:OE2	2.44	0.70
1:A:500:ASN:O	1:A:512:ARG:NH1	2.24	0.70
1:A:515:ASP:C	1:A:515:ASP:OD1	2.33	0.70
1:D:550:LEU:HA	1:D:553:LEU:CD1	2.22	0.70
1:G:550:LEU:CA	1:G:553:LEU:HD21	2.13	0.70
1:H:484:PRO:O	1:H:488:ILE:CD1	2.39	0.70
1:C:53:MET:HE2	1:C:145:ARG:HG2	1.74	0.70
1:G:550:LEU:C	1:G:553:LEU:HD22	2.15	0.70
1:H:533:GLU:OE2	3:H:801:SWA:HC8	1.92	0.70
1:B:363:SER:OG	1:B:684:GLU:OE1	2.08	0.70
1:C:363:SER:OG	1:C:684:GLU:CD	2.34	0.70
1:D:573:ILE:HD12	1:D:573:ILE:C	2.06	0.70
1:B:608:ILE:CG2	1:B:624:LEU:HD13	2.22	0.70
1:C:515:ASP:C	1:C:515:ASP:OD1	2.31	0.70
1:F:331:TYR:CE2	1:F:375:THR:HG23	2.27	0.70
1:G:442:TYR:CE1	1:G:443:GLU:CD	2.69	0.70
1:A:431:HIS:CD2	1:A:433:GLU:H	2.06	0.70
1:D:459:GLU:HG2	1:D:532:THR:HG22	1.73	0.69
1:H:442:TYR:CG	1:H:443:GLU:OE2	2.45	0.69
1:H:631:MET:HE2	1:H:631:MET:HA	1.74	0.69
1:H:472:TRP:CE3	1:H:476:ARG:CD	2.73	0.69
1:D:507:LYS:HZ1	1:D:559:MET:CE	2.04	0.69
1:F:566:SER:O	1:F:570:VAL:HG13	1.92	0.69
1:F:592[B]:MET:CA	1:F:592[B]:MET:CE	2.69	0.69
1:C:363:SER:OG	1:C:684:GLU:OE2	2.10	0.69
1:D:685:ASN:HD21	1:D:687:ASN:H	1.40	0.69
1:F:364:VAL:HG12	1:F:368:MET:HE3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:HIS:CD2	1:B:433:GLU:H	2.09	0.69
1:B:547:PRO:O	1:B:551:ILE:HG13	1.93	0.69
1:G:314:ARG:NE	1:G:343:ASP:OD2	2.19	0.69
1:A:188:ASN:HD22	1:A:190:GLY:H	1.41	0.69
1:F:363:SER:OG	1:F:684:GLU:OE2	2.11	0.69
1:F:515:ASP:OD1	1:F:517:THR:OG1	2.10	0.69
1:H:53:MET:HE2	1:H:145:ARG:HG2	1.74	0.69
1:H:428:GLU:HA	1:H:442:TYR:CD2	2.27	0.69
1:B:331:TYR:CZ	1:B:375:THR:HG23	2.29	0.68
1:E:706:MET:CE	1:E:741:ARG:NH2	2.47	0.68
1:H:472:TRP:CE2	1:H:476:ARG:HD2	2.19	0.68
1:B:592[B]:MET:HE2	1:B:631:MET:HE2	1.57	0.68
1:E:744:LYS:HB2	1:E:747:ASP:OD2	1.93	0.68
1:F:363:SER:OG	1:F:684:GLU:CD	2.37	0.68
1:G:550:LEU:O	1:G:553:LEU:HD22	1.93	0.68
1:E:188:ASN:HD22	1:E:190:GLY:H	1.42	0.68
1:F:415:ASP:OD2	1:F:418:THR:OG1	2.11	0.68
1:H:252:SER:HG	1:H:318:GLU:CD	1.98	0.68
1:D:597:TYR:OH	1:D:599:HIS:HD2	1.76	0.68
1:F:157:ASP:OD1	1:F:238:LYS:CE	2.39	0.68
1:A:745:GLU:C	1:A:745:GLU:OE1	2.37	0.68
1:H:564:MET:HE1	1:H:610:LEU:CB	2.22	0.68
1:C:631:MET:HE2	1:C:631:MET:HA	1.74	0.68
1:E:533:GLU:OE2	3:E:801:SWA:HC8	1.93	0.68
1:G:188:ASN:HD22	1:G:190:GLY:H	1.42	0.68
1:G:405:ASP:CG	1:G:409:LYS:NZ	2.51	0.68
1:C:331:TYR:CZ	1:C:375:THR:HG23	2.29	0.67
1:G:515:ASP:OD1	1:G:517:THR:OG1	2.08	0.67
1:D:364:VAL:HG12	1:D:368:MET:HE3	1.74	0.67
1:D:525:LEU:HD13	1:D:573:ILE:HG23	1.75	0.67
1:E:417:LYS:O	1:E:421:GLU:HG3	1.93	0.67
1:E:564:MET:HE1	1:E:610:LEU:HB2	1.75	0.67
1:H:550:LEU:HD12	1:H:553:LEU:HD12	1.76	0.67
1:H:415:ASP:CG	1:H:418:THR:OG1	2.37	0.67
1:C:564:MET:HE1	1:C:610:LEU:HB2	1.76	0.67
1:H:22:TRP:H	1:H:283:ASN:ND2	1.90	0.67
1:H:472:TRP:CD2	1:H:476:ARG:CG	2.77	0.67
1:E:358:ASN:ND2	1:E:365:ASN:HD22	1.92	0.67
1:F:608:ILE:CG2	1:F:624:LEU:HD13	2.25	0.67
1:D:431:HIS:CD2	1:D:433:GLU:H	2.09	0.67
1:G:549:GLY:O	1:G:553:LEU:HD22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:SER:HB3	5:B:2001:HOH:O	1.95	0.67
1:B:167:ASP:O	1:B:168:LYS:HB2	1.95	0.67
1:A:22:TRP:H	1:A:283:ASN:ND2	1.93	0.66
1:D:503:ASP:C	1:D:503:ASP:OD1	2.39	0.66
1:C:431:HIS:CD2	1:C:433:GLU:H	2.13	0.66
1:C:755:GLU:O	1:C:756:LEU:C	2.37	0.66
1:H:721:GLU:OE2	1:H:721:GLU:N	2.26	0.66
1:G:431:HIS:CD2	1:G:433:GLU:H	2.14	0.66
1:H:502:PHE:CE1	1:H:553:LEU:HB2	2.30	0.66
1:A:358:ASN:ND2	1:A:365:ASN:HD22	1.92	0.66
1:B:315:LYS:HZ1	4:B:804:GOL:H32	1.59	0.66
1:F:188:ASN:HD22	1:F:190:GLY:H	1.43	0.66
1:G:685:ASN:C	1:G:685:ASN:ND2	2.44	0.66
1:H:472:TRP:CZ3	1:H:476:ARG:HD3	2.31	0.66
1:G:507:LYS:HZ1	1:G:559:MET:CE	1.80	0.66
1:A:459:GLU:HG2	1:A:532:THR:HG22	1.78	0.66
1:C:608:ILE:CG2	1:C:624:LEU:HD13	2.26	0.66
1:D:145:ARG:NH2	1:D:317:TYR:O	2.22	0.66
1:D:167:ASP:O	1:D:168:LYS:HB2	1.94	0.66
1:F:631:MET:HE2	1:F:631:MET:HA	1.78	0.66
1:B:459:GLU:HG2	1:B:532:THR:HG22	1.77	0.66
1:G:550:LEU:CA	1:G:553:LEU:HD22	2.23	0.66
1:H:526:LYS:HA	1:H:575:ASP:HB3	1.78	0.66
1:B:546:ASP:N	1:B:547:PRO:HD3	2.11	0.66
1:E:745:GLU:OE1	1:E:745:GLU:C	2.39	0.66
1:G:608:ILE:CG2	1:G:624:LEU:HD13	2.26	0.66
1:H:188:ASN:HD22	1:H:190:GLY:H	1.43	0.66
1:E:206:LYS:HD2	1:E:237:PHE:CD1	2.30	0.66
1:C:573:ILE:CD1	1:C:574:PHE:N	2.46	0.65
1:D:515:ASP:C	1:D:515:ASP:OD1	2.37	0.65
1:F:358:ASN:HD21	1:F:365:ASN:HD22	1.43	0.65
1:G:550:LEU:HD12	1:G:553:LEU:HD23	1.78	0.65
1:B:506:SER:O	1:B:507:LYS:HB2	1.94	0.65
1:A:20:LYS:HG3	1:A:22:TRP:CH2	2.30	0.65
1:B:22:TRP:H	1:B:283:ASN:HD21	1.43	0.65
1:A:485:LYS:H	1:A:485:LYS:CD	2.09	0.65
1:B:358:ASN:HD21	1:B:365:ASN:HD22	1.43	0.65
1:B:526:LYS:HA	1:B:575:ASP:HB3	1.79	0.65
1:D:397:ASN:ND2	1:D:439:ARG:HE	1.93	0.65
1:F:415:ASP:CG	1:F:418:THR:OG1	2.39	0.65
1:G:331:TYR:CE2	1:G:375:THR:HG23	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:GLU:OE2	1:C:315:LYS:NZ	2.25	0.65
1:F:483:ARG:O	1:F:488:ILE:HD11	1.95	0.65
1:D:358:ASN:ND2	1:D:365:ASN:HD22	1.95	0.65
1:H:339:TYR:CE1	1:H:367:GLU:CG	2.79	0.65
1:H:347:TRP:HZ3	3:H:801:SWA:C7	2.10	0.65
1:F:350:PHE:C	1:F:350:PHE:CD2	2.75	0.65
1:H:472:TRP:CE3	1:H:476:ARG:CG	2.80	0.65
1:D:417:LYS:NZ	1:D:421:GLU:OE2	2.19	0.64
1:F:84:GLN:HG3	1:F:90:ASN:C	2.22	0.64
1:C:397:ASN:HD22	1:C:439:ARG:NE	1.92	0.64
1:G:681:LEU:HD23	1:G:681:LEU:N	2.10	0.64
1:B:631:MET:HE2	1:B:631:MET:HA	1.80	0.64
1:C:706:MET:CE	1:C:741:ARG:HH22	2.07	0.64
1:E:597:TYR:OH	1:E:599:HIS:HD2	1.80	0.64
1:F:472:TRP:CZ2	1:F:476:ARG:HD3	2.33	0.64
1:F:507:LYS:CE	1:F:559:MET:HE2	2.28	0.64
1:H:448:LEU:HD22	1:H:448:LEU:N	2.12	0.64
1:A:157:ASP:OD1	1:A:238:LYS:HE3	1.97	0.64
1:G:533:GLU:OE2	3:G:801:SWA:HC91	1.98	0.64
1:G:745:GLU:C	1:G:745:GLU:OE1	2.40	0.64
1:H:500:ASN:O	1:H:512:ARG:NH1	2.28	0.64
1:D:510:ARG:NH2	1:D:519:GLN:O	2.25	0.64
1:H:745:GLU:OE1	1:H:745:GLU:C	2.40	0.64
1:B:507:LYS:HE3	1:B:559[B]:MET:HE2	1.79	0.64
1:D:443:GLU:N	1:D:443:GLU:OE2	2.27	0.64
1:F:685:ASN:C	1:F:685:ASN:ND2	2.45	0.64
1:H:525:LEU:HD13	1:H:573:ILE:HG23	1.78	0.64
1:C:592[B]:MET:HE2	1:C:631:MET:HE1	0.64	0.64
1:C:525:LEU:HD13	1:C:573:ILE:HG23	1.79	0.63
1:D:415:ASP:CG	1:D:418:THR:OG1	2.41	0.63
1:H:667:ASP:OD2	1:H:719:ARG:HG2	1.98	0.63
1:A:608:ILE:HG21	1:A:624:LEU:HD13	1.81	0.63
1:B:573:ILE:HD12	1:B:574:PHE:N	2.13	0.63
1:C:188:ASN:HD22	1:C:190:GLY:H	1.46	0.63
1:E:20:LYS:O	1:E:22:TRP:CZ3	2.51	0.63
1:E:573:ILE:CD1	1:E:574:PHE:N	2.47	0.63
1:G:364:VAL:HG12	1:G:368:MET:HE3	1.79	0.63
1:H:681:LEU:HD23	1:H:681:LEU:N	2.12	0.63
1:B:685:ASN:C	1:B:685:ASN:ND2	2.55	0.63
1:H:443:GLU:CD	1:H:443:GLU:H	2.07	0.63
1:A:592:MET:SD	1:A:631:MET:HE1	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:565:ASP:OD2	1:G:619:LYS:NZ	2.31	0.63
1:H:320:ASP:C	1:H:320:ASP:OD1	2.42	0.63
1:A:592:MET:HE3	1:A:640:CYS:HB2	1.81	0.63
1:A:597:TYR:OH	1:A:599:HIS:HD2	1.82	0.63
1:B:109:GLU:HB2	1:E:110:LYS:HZ1	1.63	0.63
1:B:331:TYR:CE2	1:B:375:THR:HG23	2.34	0.63
1:D:375:THR:HG21	1:D:383:PRO:HD3	1.79	0.63
1:E:483:ARG:O	1:E:488:ILE:HD11	1.99	0.63
1:F:431:HIS:CD2	1:F:433:GLU:H	2.15	0.63
1:B:706:MET:CE	1:B:741:ARG:HH22	2.10	0.63
1:F:22:TRP:H	1:F:283:ASN:ND2	1.96	0.63
1:G:342:THR:O	1:G:343:ASP:HB2	1.97	0.63
1:G:631:MET:HE2	1:G:631:MET:HA	1.80	0.63
1:H:685:ASN:HD21	1:H:687:ASN:H	1.47	0.63
1:D:506:SER:O	1:D:507:LYS:HB2	1.99	0.63
1:F:483:ARG:HB3	1:F:487:GLU:OE2	1.98	0.63
1:H:431:HIS:CD2	1:H:433:GLU:H	2.15	0.63
1:C:459:GLU:HG2	1:C:532:THR:HG22	1.80	0.63
1:B:53:MET:HE2	1:B:145:ARG:HG2	1.80	0.62
1:C:331:TYR:CE2	1:C:375:THR:HG23	2.34	0.62
1:D:211:LYS:NZ	1:D:222:ASN:OD1	2.32	0.62
1:A:566:SER:O	1:A:570:VAL:HG13	1.99	0.62
1:C:533:GLU:OE2	3:C:801:SWA:HC8	2.00	0.62
1:E:431:HIS:CD2	1:E:433:GLU:H	2.17	0.62
1:G:472:TRP:CZ2	1:G:476:ARG:HD3	2.34	0.62
1:G:597:TYR:OH	1:G:599:HIS:HD2	1.82	0.62
1:B:472:TRP:CZ2	1:B:476:ARG:HD3	2.34	0.62
1:C:358:ASN:ND2	1:C:365:ASN:HD22	1.96	0.62
1:D:493:LYS:HE2	5:D:2075:HOH:O	1.99	0.62
1:E:211:LYS:NZ	1:E:222:ASN:OD1	2.31	0.62
1:H:361:TYR:N	1:H:362:PRO:CD	2.63	0.62
1:A:631:MET:HA	1:A:631:MET:HE2	1.81	0.62
1:E:685:ASN:C	1:E:685:ASN:ND2	2.49	0.62
1:C:566:SER:O	1:C:570:VAL:HG13	1.99	0.62
1:G:503:ASP:CG	1:G:506:SER:HG	2.06	0.62
1:B:745:GLU:C	1:B:745:GLU:OE1	2.42	0.62
1:C:363:SER:OG	1:C:684:GLU:OE1	2.17	0.62
1:C:745:GLU:C	1:C:745:GLU:OE1	2.43	0.62
1:F:347:TRP:CZ3	3:F:801:SWA:HC7	2.34	0.62
1:G:354:PHE:CD2	1:G:402:ILE:CD1	2.83	0.62
1:F:685:ASN:HD21	1:F:687:ASN:H	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:397:ASN:ND2	1:H:439:ARG:HE	1.97	0.61
1:B:361:TYR:N	1:B:362:PRO:CD	2.62	0.61
1:D:677:LYS:NZ	1:D:696:ASN:O	2.33	0.61
1:E:483:ARG:HB3	1:E:487:GLU:OE2	2.00	0.61
1:F:472:TRP:O	1:F:476:ARG:HG2	2.00	0.61
1:H:485:LYS:N	1:H:488:ILE:HD12	2.16	0.61
1:D:452:PRO:HB2	1:D:455:VAL:HG13	1.83	0.61
1:H:472:TRP:CZ3	1:H:476:ARG:NE	2.60	0.61
1:A:565:ASP:OD2	1:A:619:LYS:NZ	2.34	0.61
1:B:403:LEU:HD22	1:B:419:LEU:HD13	1.83	0.61
1:E:496:MET:HE2	1:E:752:PHE:CE2	2.36	0.61
1:G:685:ASN:HD21	1:G:687:ASN:H	1.46	0.61
1:C:254:ILE:O	4:C:803:GOL:C3	2.48	0.61
1:F:320:ASP:C	1:F:320:ASP:OD1	2.44	0.61
1:F:745:GLU:C	1:F:745:GLU:OE1	2.44	0.61
1:H:428:GLU:O	1:H:442:TYR:CZ	2.53	0.61
1:B:472:TRP:O	1:B:476:ARG:HG2	2.01	0.61
1:F:284:GLN:HG2	5:F:2029:HOH:O	2.00	0.61
1:H:270:ASN:OD1	1:H:273:GLN:HG3	2.01	0.61
1:C:597:TYR:OH	1:C:599:HIS:HD2	1.84	0.60
1:H:592:MET:HA	1:H:592:MET:CE	2.18	0.60
1:H:597:TYR:OH	1:H:599:HIS:HD2	1.84	0.60
1:B:565:ASP:OD2	1:B:619:LYS:NZ	2.34	0.60
1:D:417:LYS:O	1:D:421:GLU:HG3	2.01	0.60
1:E:547:PRO:HG2	1:E:613:TYR:CD2	2.37	0.60
1:G:503:ASP:CG	1:G:506:SER:OG	2.43	0.60
1:B:744:LYS:HB2	1:B:747:ASP:OD2	2.02	0.60
1:E:565:ASP:OD2	1:E:619:LYS:NZ	2.34	0.60
1:H:480:GLU:C	1:H:481:LEU:HD23	2.26	0.60
1:B:397:ASN:ND2	1:B:439:ARG:HE	1.99	0.60
1:C:364:VAL:HG12	1:C:368:MET:HE3	1.82	0.60
1:F:715:LYS:HE3	1:F:717:TYR:OH	2.00	0.60
1:A:472:TRP:O	1:A:476:ARG:HG2	2.02	0.60
1:B:525:LEU:HD13	1:B:573:ILE:HG23	1.84	0.60
1:D:505:GLU:HG2	1:D:506:SER:N	2.16	0.60
1:E:643:GLU:OE2	1:E:649:SER:CB	2.49	0.60
1:F:526:LYS:HA	1:F:575:ASP:HB3	1.84	0.60
1:G:316:PHE:CE2	1:G:330:PRO:HG3	2.37	0.60
1:H:546:ASP:N	1:H:547:PRO:HD3	2.16	0.60
1:H:550:LEU:HA	1:H:553:LEU:HD12	1.84	0.60
1:G:147:VAL:HG22	1:G:148:LEU:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:476:ARG:CB	1:H:476:ARG:HH11	2.08	0.60
1:C:685:ASN:C	1:C:685:ASN:ND2	2.52	0.60
1:D:721:GLU:HB2	5:D:2106:HOH:O	1.99	0.60
1:E:431:HIS:CD2	1:E:434:VAL:H	2.19	0.60
1:F:680:THR:C	1:F:681:LEU:HD23	2.27	0.60
1:B:500:ASN:O	1:B:512:ARG:NH1	2.33	0.60
1:D:415:ASP:OD2	1:D:418:THR:OG1	2.20	0.60
1:G:165:ALA:O	1:G:166:PHE:HB2	2.01	0.60
1:H:720:HIS:NE2	1:H:724:PHE:CE2	2.69	0.60
1:A:459:GLU:O	1:A:463:ARG:HG3	2.02	0.60
1:F:721:GLU:N	1:F:721:GLU:CD	2.59	0.60
1:G:483:ARG:HB3	1:G:487:GLU:OE2	2.02	0.60
1:D:631:MET:HE2	1:D:631:MET:HA	1.83	0.59
1:A:564:MET:HE1	1:A:610:LEU:CB	2.32	0.59
1:C:415:ASP:CG	1:C:418:THR:HG1	2.10	0.59
1:G:320:ASP:C	1:G:320:ASP:OD1	2.44	0.59
1:H:320:ASP:OD1	1:H:322:ASN:N	2.34	0.59
1:H:497:ASN:HA	1:H:500:ASN:ND2	2.16	0.59
1:B:573:ILE:CD1	1:B:574:PHE:H	2.13	0.59
1:A:101:VAL:HG13	1:A:156:ASN:ND2	2.18	0.59
1:G:604:ILE:O	1:G:604:ILE:HG23	2.02	0.59
1:A:320:ASP:OD1	1:A:320:ASP:C	2.44	0.59
1:B:238:LYS:HE2	5:B:2032:HOH:O	2.02	0.59
1:B:592[B]:MET:SD	1:B:631:MET:HE1	2.34	0.59
1:C:709:ASN:HD21	1:C:727:GLY:HA3	1.67	0.59
1:H:717:TYR:O	1:H:718:LEU:HD23	2.03	0.59
1:H:752:PHE:O	1:H:755:GLU:CB	2.51	0.59
1:D:472:TRP:O	1:D:476:ARG:HG2	2.01	0.59
1:F:565:ASP:OD2	1:F:619:LYS:NZ	2.36	0.59
1:C:738:ASN:C	1:C:738:ASN:OD1	2.46	0.59
1:H:443:GLU:CD	1:H:443:GLU:N	2.60	0.59
1:A:363:SER:OG	1:A:684:GLU:OE2	2.20	0.59
1:E:472:TRP:O	1:E:476:ARG:HG2	2.02	0.59
1:G:443:GLU:CD	1:G:443:GLU:H	2.10	0.59
1:C:472:TRP:O	1:C:476:ARG:HG2	2.02	0.58
1:D:483:ARG:HB3	1:D:487:GLU:OE2	2.03	0.58
1:A:361:TYR:N	1:A:362:PRO:CD	2.65	0.58
1:B:484:PRO:HB3	1:B:486:LYS:NZ	2.18	0.58
1:G:500:ASN:O	1:G:512:ARG:NH1	2.35	0.58
1:G:515:ASP:OD1	1:G:515:ASP:C	2.44	0.58
1:A:358:ASN:HD21	1:A:365:ASN:HD22	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:HIS:HE1	5:A:2117:HOH:O	1.85	0.58
1:C:546:ASP:CG	1:C:753:SER:OG	2.45	0.58
1:E:331:TYR:CZ	1:E:375:THR:HG23	2.38	0.58
1:A:63:MET:HG3	1:A:166:PHE:CE2	2.38	0.58
1:B:320:ASP:C	1:B:320:ASP:OD1	2.46	0.58
1:C:153:PHE:CE1	1:C:159:SER:HB3	2.38	0.58
1:C:483:ARG:O	1:C:488:ILE:HD11	2.03	0.58
1:F:721:GLU:CD	1:F:721:GLU:H	2.11	0.58
1:G:21:ASP:O	1:G:24:GLN:HG2	2.03	0.58
1:A:431:HIS:CD2	1:A:434:VAL:H	2.22	0.58
1:B:507:LYS:NZ	1:B:559[B]:MET:HE2	2.18	0.58
1:A:483:ARG:O	1:A:488:ILE:HD11	2.04	0.58
1:E:631:MET:HE2	1:E:631:MET:HA	1.85	0.58
1:F:206:LYS:HD2	1:F:237:PHE:CD1	2.38	0.58
1:G:167:ASP:OD1	1:G:167:ASP:C	2.47	0.58
1:G:564:MET:HE1	1:G:610:LEU:CB	2.33	0.58
1:B:507:LYS:CE	1:B:559[B]:MET:HE2	2.34	0.58
1:B:738:ASN:C	1:B:738:ASN:OD1	2.46	0.58
1:A:472:TRP:CZ2	1:A:476:ARG:HD3	2.39	0.58
1:G:30:MET:HE3	1:G:633:THR:O	2.03	0.58
1:G:431:HIS:CD2	1:G:434:VAL:H	2.22	0.58
1:G:738:ASN:C	1:G:738:ASN:OD1	2.47	0.58
1:E:500:ASN:O	1:E:512:ARG:NH1	2.36	0.58
1:F:592[B]:MET:CG	1:F:631:MET:HE1	2.32	0.58
1:A:347:TRP:CZ3	3:A:801:SWA:HC7	2.39	0.57
1:B:157:ASP:OD1	1:B:238:LYS:CE	2.47	0.57
1:E:515:ASP:OD1	1:E:516:GLY:N	2.37	0.57
1:E:680:THR:C	1:E:681:LEU:HD23	2.29	0.57
1:C:500:ASN:O	1:C:512:ARG:NH1	2.35	0.57
1:D:431:HIS:CD2	1:D:434:VAL:H	2.22	0.57
1:E:53:MET:HE2	1:E:145:ARG:HG2	1.86	0.57
1:H:60:THR:O	1:H:77:ARG:NH1	2.37	0.57
1:F:153:PHE:CE1	1:F:159:SER:HB3	2.38	0.57
1:G:502:PHE:C	1:G:502:PHE:CD2	2.81	0.57
1:H:475:TYR:CZ	1:H:479:LYS:HD3	2.39	0.57
1:H:515:ASP:OD1	1:H:515:ASP:C	2.48	0.57
1:F:145:ARG:NH2	1:F:317:TYR:O	2.28	0.57
1:F:627:VAL:HG13	1:F:631:MET:HG3	1.86	0.57
1:G:417:LYS:O	1:G:421:GLU:HG3	2.05	0.57
1:H:475:TYR:CD1	1:H:475:TYR:C	2.82	0.57
1:C:415:ASP:CG	1:C:418:THR:OG1	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:ASP:C	1:E:21:ASP:OD1	2.46	0.57
1:G:361:TYR:N	1:G:362:PRO:CD	2.68	0.57
1:A:685:ASN:HD21	1:A:687:ASN:H	1.51	0.57
1:B:431:HIS:CD2	1:B:434:VAL:H	2.22	0.57
1:H:417:LYS:O	1:H:421:GLU:HG3	2.04	0.57
1:E:503:ASP:C	1:E:503:ASP:OD1	2.44	0.57
1:G:448:LEU:HD22	1:G:448:LEU:N	2.19	0.57
1:H:252:SER:OG	1:H:318:GLU:CD	2.46	0.57
1:H:706:MET:CE	1:H:741:ARG:HH22	2.08	0.57
1:B:252:SER:OG	1:B:318:GLU:CD	2.45	0.57
1:C:199:TYR:OH	4:C:803:GOL:H2	2.03	0.57
1:D:270:ASN:OD1	1:D:273:GLN:HG3	2.05	0.57
1:F:547:PRO:HG2	1:F:613:TYR:CD2	2.40	0.57
1:G:443:GLU:CD	1:G:443:GLU:N	2.62	0.57
1:G:573:ILE:CD1	1:G:574:PHE:N	2.48	0.57
1:G:750:TYR:C	1:G:750:TYR:CD2	2.83	0.57
1:A:507:LYS:HZ2	1:A:559:MET:CE	1.96	0.57
1:D:358:ASN:HD21	1:D:365:ASN:HD22	1.52	0.57
1:E:358:ASN:HD21	1:E:365:ASN:HD22	1.53	0.57
1:G:350:PHE:C	1:G:350:PHE:CD2	2.83	0.57
1:G:717:TYR:O	1:G:718:LEU:HD23	2.04	0.57
1:H:550:LEU:HA	1:H:553:LEU:CD1	2.35	0.57
1:C:22:TRP:H	1:C:283:ASN:HD21	1.52	0.56
1:F:500:ASN:O	1:F:512:ARG:NH1	2.36	0.56
1:H:365:ASN:O	1:H:368:MET:HB2	2.05	0.56
1:H:431:HIS:CD2	1:H:434:VAL:H	2.23	0.56
1:H:459:GLU:HG2	1:H:532:THR:HG22	1.87	0.56
1:H:604:ILE:HG23	1:H:604:ILE:O	2.04	0.56
1:F:431:HIS:CD2	1:F:434:VAL:H	2.23	0.56
1:G:354:PHE:CD2	1:G:402:ILE:HD12	2.39	0.56
1:H:555:GLY:O	1:H:559:MET:HE2	2.03	0.56
1:H:573:ILE:CD1	1:H:574:PHE:N	2.51	0.56
1:H:602:GLN:NE2	1:H:644:ASP:OD2	2.38	0.56
1:A:364:VAL:HG12	1:A:368:MET:HE3	1.85	0.56
1:A:706:MET:CE	1:A:741:ARG:HH22	2.13	0.56
1:C:483:ARG:HB3	1:C:487:GLU:OE2	2.05	0.56
1:C:588:GLU:C	1:C:592[A]:MET:HE3	2.31	0.56
1:C:704:ASP:OD1	1:C:736:ARG:NH2	2.34	0.56
1:D:206:LYS:HD2	1:D:237:PHE:CD1	2.40	0.56
1:E:459:GLU:HG2	1:E:532:THR:HG22	1.87	0.56
1:F:700:ASN:ND2	1:F:735:ASN:HB3	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:MET:HE3	1:H:633:THR:O	2.05	0.56
1:B:481:LEU:HD13	1:B:481:LEU:N	2.20	0.56
1:D:412:LYS:HA	5:D:2063:HOH:O	2.05	0.56
1:H:22:TRP:H	1:H:283:ASN:HD21	1.53	0.56
1:H:175:ILE:O	1:H:175:ILE:HG22	2.05	0.56
1:A:709:ASN:HD21	1:A:727:GLY:HA3	1.71	0.56
1:C:564:MET:HE1	1:C:610:LEU:CB	2.35	0.56
1:D:503:ASP:CG	1:D:506:SER:OG	2.49	0.56
1:E:270:ASN:OD1	1:E:273:GLN:HG3	2.06	0.56
1:H:443:GLU:OE2	1:H:443:GLU:N	2.39	0.56
1:A:331:TYR:CZ	1:A:375:THR:HG23	2.41	0.56
1:D:60:THR:O	1:D:77:ARG:NH1	2.39	0.56
1:E:415:ASP:CG	1:E:418:THR:HG1	1.96	0.56
1:B:481:LEU:N	1:B:481:LEU:CD1	2.68	0.56
1:F:738:ASN:C	1:F:738:ASN:OD1	2.48	0.56
1:H:475:TYR:CD1	1:H:476:ARG:N	2.74	0.56
1:B:364:VAL:HG12	1:B:368:MET:HE3	1.87	0.55
1:G:709:ASN:HD21	1:G:727:GLY:HA3	1.71	0.55
1:B:477:LEU:HG	1:B:481:LEU:HD22	1.89	0.55
1:C:270:ASN:OD1	1:C:273:GLN:HG3	2.06	0.55
1:G:270:ASN:OD1	1:G:273:GLN:HG3	2.06	0.55
1:H:347:TRP:O	1:H:351:ARG:NH2	2.39	0.55
1:H:738:ASN:C	1:H:738:ASN:OD1	2.49	0.55
1:C:744:LYS:HB2	1:C:747:ASP:OD2	2.06	0.55
1:D:153:PHE:CE1	1:D:159:SER:HB3	2.41	0.55
1:G:347:TRP:CZ3	3:G:801:SWA:HC92	2.41	0.55
1:H:555:GLY:C	1:H:559:MET:HE3	2.31	0.55
1:B:415:ASP:CG	1:B:418:THR:OG1	2.50	0.55
1:B:547:PRO:HB2	1:B:613:TYR:CD2	2.42	0.55
1:G:336:LEU:HB3	1:G:337:PRO:HD2	1.88	0.55
1:F:349:THR:HG22	1:F:353:LEU:CB	2.36	0.55
1:F:700:ASN:HD22	1:F:735:ASN:HB3	1.71	0.55
1:H:317:TYR:CE2	1:H:339:TYR:HD1	2.24	0.55
1:C:515:ASP:OD1	1:C:516:GLY:N	2.40	0.55
1:E:526:LYS:HA	1:E:575:ASP:HB3	1.88	0.55
1:G:428:GLU:HA	1:G:442:TYR:CD2	2.41	0.55
1:A:62:LYS:HE3	1:A:109:GLU:OE2	2.07	0.55
1:F:270:ASN:OD1	1:F:273:GLN:HG3	2.07	0.55
1:A:176:PRO:HD2	1:A:177:GLU:OE1	2.05	0.55
1:C:328:TYR:CE1	4:C:803:GOL:H11	2.41	0.55
1:C:428:GLU:HA	1:C:442:TYR:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:515:ASP:OD1	1:F:515:ASP:C	2.49	0.55
1:G:60:THR:O	1:G:77:ARG:NH1	2.39	0.55
1:H:504:LYS:H	1:H:504:LYS:HD2	1.70	0.55
1:A:22:TRP:H	1:A:283:ASN:HD21	1.53	0.55
1:B:573:ILE:CD1	5:B:2078:HOH:O	2.20	0.55
1:C:431:HIS:CD2	1:C:432:PRO:HD2	2.41	0.55
1:H:363:SER:N	1:H:684:GLU:OE1	2.38	0.55
1:D:744:LYS:HB2	1:D:747:ASP:OD2	2.07	0.55
1:F:363:SER:OG	1:F:684:GLU:OE1	2.25	0.55
1:A:526:LYS:HA	1:A:575:ASP:HB3	1.89	0.54
1:C:153:PHE:CD1	1:C:159:SER:HB3	2.42	0.54
1:C:453:TYR:CE1	1:C:519:GLN:HG3	2.42	0.54
1:E:571:PRO:HB3	1:F:135:ASP:OD2	2.06	0.54
1:E:573:ILE:CD1	5:E:2068:HOH:O	2.54	0.54
1:F:597:TYR:OH	1:F:599:HIS:HD2	1.89	0.54
1:F:681:LEU:HD23	1:F:681:LEU:N	2.23	0.54
1:G:101:VAL:HG13	1:G:156:ASN:ND2	2.22	0.54
1:H:347:TRP:CZ3	1:H:394:MET:HE2	2.42	0.54
1:H:565:ASP:OD2	1:H:619:LYS:NZ	2.41	0.54
1:A:363:SER:OG	1:A:684:GLU:CD	2.49	0.54
1:B:564:MET:HE1	1:B:610:LEU:CB	2.37	0.54
1:D:109:GLU:HB3	5:D:2013:HOH:O	2.06	0.54
1:D:505:GLU:CG	1:D:506:SER:N	2.69	0.54
1:D:526:LYS:HA	1:D:575:ASP:HB3	1.87	0.54
1:D:738:ASN:C	1:D:738:ASN:OD1	2.49	0.54
1:B:455:VAL:O	1:B:456:LYS:HB2	2.07	0.54
1:D:750:TYR:C	1:D:750:TYR:CD2	2.85	0.54
1:A:496[B]:MET:HE3	1:A:499:LYS:NZ	2.23	0.54
1:F:165:ALA:O	1:F:166:PHE:HB2	2.06	0.54
1:F:717:TYR:O	1:F:718:LEU:HD23	2.07	0.54
1:B:597:TYR:OH	1:B:599:HIS:HD2	1.90	0.54
1:C:415:ASP:OD2	1:C:418:THR:OG1	2.24	0.54
1:G:395:VAL:CG1	1:G:463:ARG:CZ	2.82	0.54
1:G:549:GLY:O	1:G:553:LEU:HD21	2.06	0.54
1:H:347:TRP:CE3	1:H:394:MET:HE2	2.42	0.54
1:C:431:HIS:CD2	1:C:434:VAL:H	2.25	0.54
1:D:709:ASN:HD21	1:D:727:GLY:HA3	1.71	0.54
1:H:502:PHE:CD1	1:H:553:LEU:HD13	2.42	0.54
1:A:206:LYS:HD2	1:A:237:PHE:CD1	2.43	0.54
1:C:165:ALA:O	1:C:166:PHE:HB2	2.06	0.54
1:D:459:GLU:CG	1:D:532:THR:HG22	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ASP:OD2	1:B:418:THR:OG1	2.26	0.54
1:B:483:ARG:O	1:B:488:ILE:HD11	2.08	0.54
1:D:507:LYS:HZ1	1:D:559:MET:HE1	1.73	0.54
1:E:709:ASN:HD21	1:E:727:GLY:HA3	1.73	0.54
1:G:167:ASP:O	1:G:168:LYS:CB	2.53	0.54
1:G:175:ILE:O	1:G:175:ILE:HG22	2.07	0.54
1:G:550:LEU:C	1:G:553:LEU:CD2	2.78	0.54
1:G:663:CYS:O	1:G:666:THR:HG23	2.07	0.54
1:A:738:ASN:C	1:A:738:ASN:OD1	2.51	0.54
1:C:565:ASP:OD2	1:C:619:LYS:NZ	2.40	0.54
1:D:564:MET:HE1	1:D:610:LEU:CB	2.37	0.54
1:F:358:ASN:HD21	1:F:365:ASN:ND2	2.06	0.54
1:A:744:LYS:HB2	1:A:747:ASP:OD2	2.08	0.53
1:C:320:ASP:C	1:C:320:ASP:OD1	2.49	0.53
1:E:421:GLU:HG2	5:E:2061:HOH:O	2.08	0.53
1:B:515:ASP:OD1	1:B:516:GLY:N	2.41	0.53
1:B:604:ILE:HG23	1:B:604:ILE:O	2.08	0.53
1:B:709:ASN:HD21	1:B:727:GLY:HA3	1.74	0.53
1:G:550:LEU:O	1:G:553:LEU:CD2	2.56	0.53
1:A:485:LYS:HE2	1:A:485:LYS:CA	2.34	0.53
1:D:503:ASP:OD2	1:D:506:SER:OG	2.23	0.53
1:E:472:TRP:CZ2	1:E:476:ARG:HD3	2.43	0.53
1:E:738:ASN:C	1:E:738:ASN:OD1	2.50	0.53
1:F:60:THR:O	1:F:77:ARG:NH1	2.39	0.53
1:E:176:PRO:HD2	1:E:177:GLU:OE1	2.08	0.53
1:G:472:TRP:O	1:G:476:ARG:HG2	2.08	0.53
1:H:101:VAL:HG13	1:H:156:ASN:ND2	2.23	0.53
1:B:315:LYS:HZ3	4:B:804:GOL:H32	1.70	0.53
1:E:320:ASP:C	1:E:320:ASP:OD1	2.52	0.53
1:E:503:ASP:CG	1:E:506:SER:OG	2.51	0.53
1:F:564:MET:HE1	1:F:610:LEU:HB2	1.91	0.53
1:G:415:ASP:CG	1:G:418:THR:HG1	2.10	0.53
1:B:415:ASP:CG	1:B:418:THR:HG1	2.17	0.53
1:C:206:LYS:HD2	1:C:237:PHE:CD1	2.42	0.53
1:C:336:LEU:HB3	1:C:337:PRO:HD2	1.89	0.53
1:C:417:LYS:NZ	1:C:421:GLU:OE2	2.25	0.53
1:E:564:MET:HE1	1:E:610:LEU:CB	2.39	0.53
1:E:700:ASN:ND2	1:E:735:ASN:HB3	2.23	0.53
1:G:91:ASP:OD1	1:G:92:TYR:N	2.37	0.53
1:G:454:ASP:OD2	1:G:513:ASN:CB	2.54	0.53
1:A:597:TYR:CE2	1:A:599:HIS:HB2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:HB2	1:E:110:LYS:HZ2	1.72	0.53
1:G:459:GLU:HG2	1:G:532:THR:HG22	1.91	0.53
1:B:754:LYS:O	1:B:755:GLU:HG3	2.09	0.53
1:D:588:GLU:O	1:D:592[A]:MET:HG3	2.09	0.53
1:F:22:TRP:H	1:F:283:ASN:HD21	1.56	0.53
1:H:709:ASN:HD21	1:H:727:GLY:HA3	1.74	0.53
1:F:364:VAL:CG1	1:F:368:MET:HE3	2.39	0.53
1:G:453:TYR:CE1	1:G:519:GLN:HG3	2.44	0.53
1:H:165:ALA:O	1:H:166:PHE:HB2	2.08	0.53
1:B:503:ASP:CG	1:B:506:SER:OG	2.52	0.53
1:C:330:PRO:HB3	1:C:388:PRO:HB2	1.91	0.53
1:D:700:ASN:ND2	1:D:735:ASN:HB3	2.24	0.53
1:E:515:ASP:OD1	1:E:517:THR:OG1	2.27	0.53
1:F:332:ASN:C	1:F:332:ASN:OD1	2.52	0.53
1:G:526:LYS:HA	1:G:575:ASP:HB3	1.91	0.53
1:G:700:ASN:ND2	1:G:735:ASN:HB3	2.24	0.53
1:C:477:LEU:HG	1:C:481:LEU:HD22	1.92	0.52
1:D:570:VAL:O	1:D:570:VAL:CG2	2.56	0.52
1:E:365:ASN:O	1:E:369:GLN:HG2	2.10	0.52
1:F:330:PRO:HB3	1:F:388:PRO:HB2	1.91	0.52
1:G:348:ASP:OD2	3:G:801:SWA:HC7	2.08	0.52
1:H:519:GLN:HG2	1:H:520:SER:N	2.23	0.52
1:H:750:TYR:C	1:H:750:TYR:CD2	2.86	0.52
1:A:385:TRP:CD1	1:A:393:CYS:HB3	2.44	0.52
1:C:526:LYS:HA	1:C:575:ASP:HB3	1.90	0.52
1:F:365:ASN:O	1:F:369:GLN:HG2	2.09	0.52
1:H:476:ARG:HH11	1:H:476:ARG:HA	1.74	0.52
1:B:206:LYS:HD2	1:B:237:PHE:CD1	2.44	0.52
1:C:329:SER:OG	1:C:378:GLU:OE1	2.26	0.52
1:D:347:TRP:CZ3	3:D:801:SWA:HC7	2.44	0.52
1:H:548:GLN:NE2	1:H:552:ASP:OD1	2.43	0.52
1:A:60:THR:O	1:A:77:ARG:NH1	2.41	0.52
1:A:431:HIS:CD2	1:A:432:PRO:HD2	2.43	0.52
1:A:451:VAL:O	1:A:460:ASN:HB2	2.09	0.52
1:B:330:PRO:HB3	1:B:388:PRO:HB2	1.91	0.52
1:C:358:ASN:HD21	1:C:365:ASN:HD22	1.57	0.52
1:F:53:MET:HE2	1:F:145:ARG:HG2	1.90	0.52
1:F:573:ILE:CD1	1:F:574:PHE:N	2.52	0.52
1:F:709:ASN:HD21	1:F:727:GLY:HA3	1.73	0.52
1:F:750:TYR:C	1:F:750:TYR:CD2	2.87	0.52
1:H:415:ASP:CG	1:H:418:THR:HG1	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:PRO:HB3	1:A:388:PRO:HB2	1.92	0.52
1:B:101:VAL:HG13	1:B:156:ASN:ND2	2.24	0.52
1:B:515:ASP:OD1	1:B:517:THR:OG1	2.28	0.52
1:B:606:HIS:HB3	5:B:2097:HOH:O	2.07	0.52
4:B:803:GOL:H32	5:B:2039:HOH:O	2.09	0.52
1:D:616:GLN:HG2	1:D:618:TRP:CZ2	2.44	0.52
1:H:63:MET:HG3	1:H:166:PHE:CE2	2.45	0.52
1:A:455:VAL:O	1:A:456:LYS:HB2	2.09	0.52
1:A:608:ILE:CG2	1:A:624:LEU:HD13	2.39	0.52
1:B:176:PRO:HD2	1:B:177:GLU:OE1	2.10	0.52
1:C:101:VAL:HG13	1:C:156:ASN:ND2	2.25	0.52
1:G:526:LYS:O	1:G:535:ASN:CB	2.57	0.52
1:A:506:SER:O	1:A:507:LYS:HB2	2.09	0.52
1:D:597:TYR:CE2	1:D:599:HIS:HB2	2.45	0.52
1:A:431:HIS:HD2	1:A:433:GLU:N	2.02	0.52
1:D:431:HIS:CD2	1:D:432:PRO:HD2	2.45	0.52
1:F:407:TYR:CE1	1:F:412:LYS:HE2	2.45	0.52
1:F:431:HIS:CD2	1:F:432:PRO:HD2	2.45	0.52
1:A:412:LYS:HA	5:A:2070:HOH:O	2.10	0.52
1:C:506:SER:O	1:C:507:LYS:HB2	2.08	0.52
1:D:320:ASP:C	1:D:320:ASP:OD1	2.52	0.52
1:H:153:PHE:CE1	1:H:159:SER:HB3	2.44	0.52
1:H:431:HIS:CD2	1:H:432:PRO:HD2	2.45	0.52
1:A:165:ALA:O	1:A:166:PHE:HB2	2.09	0.52
1:A:415:ASP:OD2	1:A:418:THR:OG1	2.26	0.52
1:B:453:TYR:CE1	1:B:519:GLN:HG3	2.44	0.52
1:E:549:GLY:O	1:E:553:LEU:HG	2.09	0.52
1:H:506:SER:O	1:H:507:LYS:HB2	2.08	0.52
1:A:453:TYR:CE1	1:A:519:GLN:HG3	2.46	0.51
1:B:348:ASP:OD1	3:B:801:SWA:O1	2.13	0.51
1:H:214:VAL:N	1:H:232:GLY:O	2.41	0.51
1:A:515:ASP:OD1	1:A:516:GLY:N	2.44	0.51
1:C:685:ASN:HD21	1:C:687:ASN:H	1.56	0.51
1:D:483:ARG:O	1:D:488:ILE:HD11	2.10	0.51
1:D:515:ASP:OD1	1:D:517:THR:OG1	2.27	0.51
1:F:453:TYR:CE1	1:F:519:GLN:HG3	2.45	0.51
1:H:92:TYR:OH	1:H:343:ASP:OD2	2.22	0.51
1:H:510:ARG:NH2	1:H:519:GLN:O	2.32	0.51
1:C:320:ASP:OD1	1:C:322:ASN:N	2.41	0.51
1:E:681:LEU:HD23	1:E:681:LEU:N	2.24	0.51
1:F:361:TYR:N	1:F:362:PRO:HD3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:459:GLU:CG	1:F:532:THR:HG22	2.41	0.51
1:H:597:TYR:CE2	1:H:599:HIS:HB2	2.45	0.51
1:A:550:LEU:HD12	1:A:553:LEU:HD12	1.91	0.51
1:B:592[B]:MET:HE1	1:B:631:MET:CE	2.24	0.51
1:D:482:LYS:HE2	5:D:2070:HOH:O	2.11	0.51
1:E:431:HIS:HD2	1:E:434:VAL:H	1.56	0.51
1:E:700:ASN:HD22	1:E:735:ASN:HB3	1.76	0.51
1:E:750:TYR:C	1:E:750:TYR:CD2	2.88	0.51
1:G:358:ASN:ND2	1:G:365:ASN:HD22	2.08	0.51
1:B:153:PHE:CE1	1:B:159:SER:HB3	2.46	0.51
1:E:362:PRO:HD2	1:E:684:GLU:CD	2.36	0.51
1:G:431:HIS:CD2	1:G:432:PRO:HD2	2.45	0.51
1:G:506:SER:O	1:G:507:LYS:HB2	2.11	0.51
1:G:602:GLN:NE2	1:G:644:ASP:OD2	2.44	0.51
1:H:347:TRP:CZ3	3:H:801:SWA:C7	2.87	0.51
1:A:320:ASP:OD1	1:A:322:ASN:N	2.43	0.51
1:A:327:HIS:ND1	1:A:338:GLY:O	2.39	0.51
1:A:549:GLY:O	1:A:553:LEU:HG	2.10	0.51
1:D:442:TYR:CD1	1:D:443:GLU:OE2	2.64	0.51
1:G:597:TYR:CE2	1:G:599:HIS:HB2	2.46	0.51
1:E:22:TRP:H	1:E:283:ASN:ND2	2.08	0.51
1:F:21:ASP:OD1	1:F:22:TRP:N	2.44	0.51
1:F:320:ASP:OD1	1:F:322:ASN:N	2.39	0.51
1:G:320:ASP:OD1	1:G:322:ASN:N	2.42	0.51
1:G:547:PRO:HB2	1:G:613:TYR:CD2	2.46	0.51
1:B:358:ASN:HD21	1:B:365:ASN:ND2	2.09	0.51
1:C:663:CYS:O	1:C:666:THR:HG23	2.11	0.51
1:D:472:TRP:CZ2	1:D:476:ARG:HD3	2.46	0.51
1:A:20:LYS:HD2	1:A:20:LYS:C	2.35	0.50
1:D:175:ILE:HG22	1:D:175:ILE:O	2.11	0.50
1:D:700:ASN:HD22	1:D:735:ASN:HB3	1.76	0.50
1:F:428:GLU:HA	1:F:442:TYR:CD2	2.46	0.50
1:G:33:GLN:HG3	1:G:71:TYR:HB3	1.93	0.50
1:B:353:LEU:C	1:B:353:LEU:HD13	2.36	0.50
1:D:519:GLN:HG2	1:D:520:SER:N	2.27	0.50
1:E:257[A]:GLU:H	1:E:257[A]:GLU:CD	2.19	0.50
1:E:597:TYR:CE2	1:E:599:HIS:HB2	2.47	0.50
1:G:405:ASP:OD1	1:G:409:LYS:CE	2.58	0.50
1:E:455:VAL:O	1:E:456:LYS:HB2	2.10	0.50
1:H:336:LEU:HB3	1:H:337:PRO:HD2	1.92	0.50
1:H:663:CYS:O	1:H:666:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:CYS:O	1:A:666:THR:HG23	2.11	0.50
1:B:175:ILE:O	1:B:175:ILE:HG22	2.11	0.50
1:C:365:ASN:O	1:C:369:GLN:HG2	2.11	0.50
1:D:153:PHE:CD1	1:D:159:SER:HB3	2.46	0.50
1:D:252:SER:OG	1:D:318:GLU:OE1	2.18	0.50
1:E:331:TYR:CE2	1:E:375:THR:HG23	2.46	0.50
1:E:453:TYR:CE1	1:E:519:GLN:HG3	2.46	0.50
1:F:549:GLY:O	1:F:553:LEU:CD1	2.59	0.50
1:G:22:TRP:H	1:G:283:ASN:ND2	2.09	0.50
1:H:591:VAL:HG23	1:H:592:MET:HE3	1.94	0.50
1:C:60:THR:O	1:C:77:ARG:NH1	2.41	0.50
1:C:342:THR:O	1:C:343:ASP:HB2	2.12	0.50
1:C:361:TYR:N	1:C:362:PRO:CD	2.75	0.50
1:C:515:ASP:OD1	1:C:517:THR:OG1	2.30	0.50
1:E:336:LEU:HB3	1:E:337:PRO:HD2	1.93	0.50
1:E:503:ASP:OD2	1:E:506:SER:OG	2.25	0.50
1:F:153:PHE:CD1	1:F:159:SER:HB3	2.46	0.50
1:G:611:TYR:HB2	1:G:620:ALA:HB2	1.94	0.50
1:H:428:GLU:O	1:H:442:TYR:CE2	2.64	0.50
1:H:459:GLU:O	1:H:463:ARG:HG3	2.12	0.50
1:A:153:PHE:CE1	1:A:159:SER:HB3	2.46	0.50
1:C:385:TRP:CD1	1:C:393:CYS:HB3	2.47	0.50
1:D:546:ASP:N	1:D:547:PRO:HD3	2.27	0.50
1:F:547:PRO:HB2	1:F:613:TYR:CD2	2.47	0.50
1:F:663:CYS:O	1:F:666:THR:HG23	2.11	0.50
1:G:90:ASN:HB3	1:G:189:SER:OG	2.12	0.50
1:H:365:ASN:O	1:H:368:MET:N	2.45	0.50
1:A:90:ASN:HB3	1:A:189:SER:OG	2.12	0.50
1:A:700:ASN:ND2	1:A:735:ASN:HB3	2.27	0.50
1:C:472:TRP:CZ2	1:C:476:ARG:HD3	2.46	0.50
1:C:755:GLU:O	1:C:756:LEU:O	2.30	0.50
1:F:407:TYR:CE2	1:F:412:LYS:HD3	2.46	0.50
1:F:506:SER:O	1:F:507:LYS:HB2	2.10	0.50
1:G:213:THR:HG23	1:G:223:VAL:O	2.12	0.50
1:G:451:VAL:O	1:G:460:ASN:HB2	2.11	0.50
1:H:451:VAL:O	1:H:460:ASN:HB2	2.12	0.50
1:A:270:ASN:OD1	1:A:273:GLN:HG3	2.11	0.49
1:A:515:ASP:OD1	1:A:517:THR:OG1	2.30	0.49
1:A:558[B]:GLU:H	1:A:558[B]:GLU:CD	2.18	0.49
1:C:680:THR:C	1:C:681:LEU:HD23	2.37	0.49
1:E:459:GLU:O	1:E:463:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:431:HIS:HD2	1:H:434:VAL:H	1.61	0.49
1:D:342:THR:O	1:D:343:ASP:HB2	2.12	0.49
1:D:602:GLN:NE2	1:D:644:ASP:OD2	2.44	0.49
1:G:442:TYR:CE1	1:G:443:GLU:OE1	2.66	0.49
1:G:613:TYR:CE1	1:G:749:PRO:HG2	2.47	0.49
1:G:616:GLN:HG2	1:G:618:TRP:CZ2	2.46	0.49
1:F:451:VAL:O	1:F:460:ASN:HB2	2.11	0.49
1:F:481:LEU:N	1:F:481:LEU:CD1	2.74	0.49
1:B:397:ASN:HD22	1:B:439:ARG:NE	2.07	0.49
1:C:350:PHE:CD2	1:C:350:PHE:C	2.90	0.49
1:E:685:ASN:HD22	1:E:687:ASN:H	1.57	0.49
1:G:206:LYS:HD2	1:G:237:PHE:CD1	2.48	0.49
1:H:141:THR:C	1:H:147:VAL:HG23	2.37	0.49
1:B:503:ASP:CG	1:B:506:SER:HG	2.20	0.49
1:B:558[A]:GLU:H	1:B:558[A]:GLU:CD	2.19	0.49
1:E:153:PHE:CD1	1:E:159:SER:HB3	2.47	0.49
1:G:547:PRO:HG2	1:G:613:TYR:CD2	2.43	0.49
1:A:680:THR:C	1:A:681:LEU:HD23	2.37	0.49
1:C:555:GLY:O	1:C:559:MET:HG3	2.13	0.49
1:D:487:GLU:CD	5:D:2074:HOH:O	2.56	0.49
1:F:101:VAL:HG13	1:F:156:ASN:ND2	2.28	0.49
1:F:494:ARG:O	1:F:497:ASN:ND2	2.45	0.49
1:G:720:HIS:NE2	1:G:724:PHE:CE2	2.80	0.49
1:H:476:ARG:HH11	1:H:476:ARG:CA	2.25	0.49
1:B:663:CYS:O	1:B:666:THR:HG23	2.12	0.49
1:E:329:SER:OG	1:E:378:GLU:OE1	2.27	0.49
1:F:347:TRP:HZ3	3:F:801:SWA:HC7	1.76	0.49
1:F:472:TRP:CE2	1:F:476:ARG:HD3	2.47	0.49
1:G:153:PHE:CE1	1:G:159:SER:HB3	2.47	0.49
1:H:455:VAL:O	1:H:456:LYS:HB2	2.12	0.49
1:A:750:TYR:C	1:A:750:TYR:CD2	2.90	0.49
1:D:565:ASP:OD2	1:D:619:LYS:NZ	2.46	0.49
1:E:547:PRO:HB2	1:E:613:TYR:CD2	2.48	0.49
1:F:458:ASN:O	1:F:459:GLU:HB2	2.12	0.49
1:A:604:ILE:HG23	1:A:604:ILE:O	2.13	0.49
1:B:367:GLU:OE2	4:B:804:GOL:H31	2.13	0.49
1:B:417:LYS:O	1:B:421:GLU:HG3	2.13	0.49
1:B:428:GLU:HA	1:B:442:TYR:CD2	2.47	0.49
1:B:472:TRP:CE2	1:B:476:ARG:HD3	2.48	0.49
1:C:550:LEU:HD12	1:C:553:LEU:HD12	1.94	0.49
1:E:153:PHE:CE1	1:E:159:SER:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:385:TRP:CD1	1:F:393:CYS:HB3	2.47	0.49
1:D:451:VAL:O	1:D:460:ASN:HB2	2.12	0.48
1:D:533:GLU:OE2	3:D:801:SWA:HC8	2.13	0.48
1:E:407:TYR:CD2	1:E:412:LYS:HG2	2.48	0.48
1:H:497:ASN:C	1:H:499:LYS:N	2.69	0.48
1:G:392:GLY:HA2	1:G:436:SER:OG	2.12	0.48
1:G:407:TYR:CZ	1:G:412:LYS:HE2	2.44	0.48
1:H:700:ASN:HD22	1:H:735:ASN:HB3	1.78	0.48
1:A:20:LYS:HG3	1:A:22:TRP:CZ2	2.48	0.48
1:C:700:ASN:ND2	1:C:735:ASN:HB3	2.28	0.48
1:D:428:GLU:HA	1:D:442:TYR:CD2	2.49	0.48
1:E:459:GLU:HG2	1:E:531:PHE:O	2.13	0.48
1:G:616:GLN:HG2	1:G:618:TRP:CH2	2.49	0.48
1:E:510:ARG:NH2	1:E:519:GLN:O	2.33	0.48
1:F:597:TYR:CE2	1:F:599:HIS:HB2	2.49	0.48
1:G:494:ARG:O	1:G:497:ASN:ND2	2.46	0.48
1:G:700:ASN:HD22	1:G:735:ASN:HB3	1.77	0.48
1:B:60:THR:O	1:B:77:ARG:NH1	2.40	0.48
1:C:547:PRO:HB2	1:C:613:TYR:CD2	2.47	0.48
1:D:53:MET:CE	1:D:145:ARG:HG2	2.34	0.48
1:D:570:VAL:HG23	1:D:571:PRO:O	2.14	0.48
1:E:101:VAL:HG13	1:E:156:ASN:ND2	2.29	0.48
1:G:419:LEU:HD12	1:G:419:LEU:O	2.13	0.48
1:H:700:ASN:ND2	1:H:735:ASN:HB3	2.28	0.48
1:E:364:VAL:HG12	1:E:368:MET:HE3	1.95	0.48
1:F:448:LEU:HD22	1:F:448:LEU:N	2.29	0.48
1:H:447:LYS:HG2	1:H:448:LEU:HD22	1.96	0.48
1:C:570:VAL:O	1:C:595:GLY:HA2	2.13	0.48
1:C:597:TYR:CE2	1:C:599:HIS:HB2	2.48	0.48
1:D:529:ASP:HB3	1:D:530:ALA:H	1.48	0.48
1:A:336:LEU:HB3	1:A:337:PRO:HD2	1.95	0.48
1:B:431:HIS:CD2	1:B:432:PRO:HD2	2.49	0.48
1:C:607:MET:O	1:C:610:LEU:HB2	2.14	0.48
1:F:461:ALA:HB3	1:F:530:ALA:O	2.14	0.48
1:G:332:ASN:C	1:G:332:ASN:OD1	2.57	0.48
1:G:385:TRP:CD1	1:G:393:CYS:HB3	2.49	0.48
1:G:407:TYR:CD1	1:G:412:LYS:HE2	2.48	0.48
1:H:141:THR:O	1:H:147:VAL:HG23	2.12	0.48
1:H:153:PHE:CD1	1:H:159:SER:HB3	2.48	0.48
1:H:611:TYR:HB2	1:H:620:ALA:HB2	1.96	0.48
1:D:176:PRO:HD2	1:D:177:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:616:GLN:HG2	1:D:618:TRP:CH2	2.49	0.48
1:E:72:THR:HG21	1:F:72:THR:HG21	1.96	0.48
1:F:533:GLU:OE2	3:F:801:SWA:HC8	2.14	0.48
1:F:586:ILE:O	1:F:590:THR:HG23	2.14	0.48
1:G:63:MET:HG3	1:G:166:PHE:CE2	2.49	0.48
1:B:459:GLU:O	1:B:463:ARG:HG3	2.14	0.48
1:B:546:ASP:N	1:B:547:PRO:CD	2.76	0.48
1:E:498:TYR:OH	1:E:546:ASP:OD2	2.29	0.48
1:E:569:ALA:O	1:F:241:LYS:NZ	2.33	0.48
1:F:533:GLU:OE2	3:F:801:SWA:C8	2.62	0.48
1:H:315:LYS:HE2	1:H:317:TYR:CZ	2.48	0.48
1:B:320:ASP:OD1	1:B:322:ASN:N	2.46	0.47
1:D:375:THR:O	1:D:379:SER:OG	2.12	0.47
1:E:616:GLN:HG2	1:E:618:TRP:CZ2	2.48	0.47
1:G:558:GLU:H	1:G:558:GLU:CD	2.22	0.47
1:H:350:PHE:CD2	1:H:351:ARG:N	2.82	0.47
1:H:502:PHE:C	1:H:502:PHE:CD2	2.92	0.47
1:C:328:TYR:CD1	4:C:803:GOL:H11	2.49	0.47
1:E:91:ASP:OD1	1:E:92:TYR:N	2.46	0.47
1:E:550:LEU:HD12	1:E:553:LEU:HD12	1.95	0.47
1:G:153:PHE:CD1	1:G:159:SER:HB3	2.49	0.47
1:A:570:VAL:O	1:A:595:GLY:HA2	2.14	0.47
1:B:486:LYS:HG2	5:B:2072:HOH:O	2.14	0.47
1:B:597:TYR:CE2	1:B:599:HIS:HB2	2.49	0.47
1:C:88:TRP:HB2	3:C:801:SWA:HC62	1.96	0.47
1:D:477:LEU:HG	1:D:481:LEU:HD22	1.96	0.47
1:E:570:VAL:O	1:E:595:GLY:HA2	2.14	0.47
1:E:745:GLU:C	1:E:745:GLU:CD	2.82	0.47
1:G:442:TYR:CD1	1:G:443:GLU:CD	2.92	0.47
1:H:95:PHE:HB2	1:H:164:ASP:O	2.14	0.47
1:A:63:MET:HG3	1:A:166:PHE:CD2	2.49	0.47
1:A:459:GLU:CG	1:A:532:THR:HG22	2.44	0.47
1:A:602:GLN:NE2	1:A:644:ASP:OD2	2.47	0.47
1:B:607:MET:O	1:B:607:MET:HG2	2.13	0.47
1:B:616:GLN:HG2	1:B:618:TRP:CZ2	2.49	0.47
1:C:592[B]:MET:CE	1:C:631:MET:HE3	2.11	0.47
1:D:272:GLU:HG3	4:D:802:GOL:C3	2.40	0.47
1:E:611:TYR:HB2	1:E:620:ALA:HB2	1.96	0.47
1:G:176:PRO:HD2	1:G:177:GLU:OE1	2.13	0.47
1:G:623:TRP:O	1:G:626:GLN:HB2	2.14	0.47
1:H:546:ASP:N	1:H:547:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:HB3	1:B:337:PRO:HD2	1.95	0.47
1:C:451:VAL:O	1:C:460:ASN:HB2	2.14	0.47
1:F:342:THR:O	1:F:343:ASP:HB2	2.13	0.47
1:A:627:VAL:HG13	1:A:631:MET:HG3	1.97	0.47
1:B:602:GLN:NE2	1:B:644:ASP:OD2	2.48	0.47
1:C:426:GLY:O	1:C:439:ARG:HG3	2.14	0.47
1:C:610:LEU:HD12	1:C:610:LEU:HA	1.71	0.47
1:D:611:TYR:HB2	1:D:620:ALA:HB2	1.96	0.47
1:E:320:ASP:OD1	1:E:322:ASN:N	2.47	0.47
1:E:623:TRP:O	1:E:626:GLN:HB2	2.15	0.47
1:F:616:GLN:HG2	1:F:618:TRP:CZ2	2.50	0.47
1:F:685:ASN:HD22	1:F:687:ASN:H	1.59	0.47
1:G:431:HIS:HD2	1:G:434:VAL:H	1.61	0.47
1:H:570:VAL:HG23	1:H:571:PRO:O	2.15	0.47
1:B:84:GLN:HG3	1:B:90:ASN:C	2.40	0.47
1:B:431:HIS:HD2	1:B:434:VAL:H	1.63	0.47
1:B:431:HIS:HB3	1:B:434:VAL:O	2.14	0.47
1:C:293:GLY:HA3	1:C:677:LYS:HB2	1.97	0.47
1:E:175:ILE:O	1:E:175:ILE:HG22	2.14	0.47
1:F:407:TYR:CZ	1:F:412:LYS:HD3	2.49	0.47
1:F:481:LEU:N	1:F:481:LEU:HD13	2.29	0.47
1:G:459:GLU:O	1:G:463:ARG:HG3	2.15	0.47
1:H:494:ARG:O	1:H:497:ASN:ND2	2.48	0.47
1:H:519:GLN:OE1	1:H:521:PRO:O	2.32	0.47
1:B:365:ASN:O	1:B:369:GLN:HG2	2.15	0.47
1:B:750:TYR:HE1	1:B:755:GLU:OE2	1.97	0.47
1:F:529:ASP:HB3	1:F:530:ALA:H	1.54	0.47
1:G:627:VAL:HG13	1:G:631:MET:HG3	1.97	0.47
1:H:142:PRO:CA	1:H:147:VAL:HG23	2.45	0.47
1:A:175:ILE:HG22	1:A:175:ILE:O	2.15	0.47
1:A:358:ASN:HD21	1:A:365:ASN:ND2	2.13	0.47
1:A:507:LYS:NZ	1:A:554:MET:O	2.45	0.47
1:A:611:TYR:HB2	1:A:620:ALA:HB2	1.97	0.47
1:B:484:PRO:HB3	1:B:486:LYS:HE3	1.97	0.47
1:C:23:THR:HG23	1:C:283:ASN:ND2	2.30	0.47
1:C:754:LYS:C	1:C:756:LEU:H	2.22	0.47
1:D:515:ASP:CG	1:D:517:THR:HG1	2.21	0.47
1:G:442:TYR:CZ	1:G:443:GLU:CD	2.86	0.47
1:A:30:MET:HE3	1:A:633:THR:O	2.15	0.47
1:A:332:ASN:C	1:A:332:ASN:OD1	2.58	0.47
1:A:477:LEU:HG	1:A:481:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ARG:HB3	1:B:487:GLU:OE2	2.15	0.47
1:E:167:ASP:O	1:E:168:LYS:HB2	2.14	0.47
1:G:483:ARG:HH21	1:G:487:GLU:CD	2.23	0.47
1:H:240:ARG:O	1:H:241:LYS:C	2.58	0.47
1:H:689:LEU:HD22	1:H:690:VAL:N	2.29	0.47
1:A:216:ASN:HD21	1:A:230:HIS:H	1.62	0.46
1:B:59:GLN:HE21	1:B:80:LYS:HB2	1.80	0.46
1:B:559[A]:MET:HE2	1:B:559[A]:MET:HA	1.97	0.46
1:H:51:TRP:CZ2	1:H:310:LEU:HD22	2.50	0.46
1:B:448:LEU:HD22	1:B:448:LEU:N	2.31	0.46
1:C:29:LEU:HD23	1:C:45:PRO:HG3	1.97	0.46
1:C:458:ASN:O	1:C:459:GLU:HB2	2.15	0.46
1:D:459:GLU:HG2	1:D:531:PHE:O	2.15	0.46
1:D:549:GLY:O	1:D:553:LEU:HG	2.15	0.46
1:D:566:SER:HA	1:D:569:ALA:HB3	1.97	0.46
1:E:529:ASP:HB3	1:E:530:ALA:H	1.51	0.46
1:G:528:GLY:O	1:G:530:ALA:N	2.48	0.46
1:B:750:TYR:C	1:B:750:TYR:CD2	2.92	0.46
1:C:209:THR:O	1:C:209:THR:HG22	2.16	0.46
1:C:417:LYS:O	1:C:421:GLU:HG3	2.15	0.46
1:C:681:LEU:HD23	1:C:681:LEU:N	2.30	0.46
1:D:63:MET:HG3	1:D:166:PHE:CE2	2.51	0.46
1:D:167:ASP:OD1	1:D:168:LYS:HG2	2.15	0.46
1:E:20:LYS:O	1:E:22:TRP:CE3	2.69	0.46
1:F:431:HIS:HD2	1:F:434:VAL:H	1.61	0.46
1:F:689:LEU:HD22	1:F:690:VAL:N	2.30	0.46
1:G:365:ASN:O	1:G:369:GLN:HG2	2.15	0.46
1:G:405:ASP:O	1:G:409:LYS:HG3	2.15	0.46
1:G:717:TYR:C	1:G:718:LEU:HD23	2.40	0.46
1:H:736:ARG:NH1	1:H:736:ARG:CG	2.65	0.46
1:A:685:ASN:HD22	1:A:687:ASN:H	1.59	0.46
1:A:700:ASN:HD22	1:A:735:ASN:HB3	1.79	0.46
1:B:361:TYR:N	1:B:362:PRO:HD3	2.29	0.46
1:B:700:ASN:ND2	1:B:735:ASN:HB3	2.30	0.46
1:E:30:MET:HE3	1:E:633:THR:O	2.15	0.46
1:E:330:PRO:HB3	1:E:388:PRO:HB2	1.98	0.46
1:F:336:LEU:HB3	1:F:337:PRO:HD2	1.97	0.46
1:A:157:ASP:OD1	1:A:238:LYS:CE	2.64	0.46
1:A:210:TYR:CD1	1:A:210:TYR:C	2.93	0.46
1:B:627:VAL:HG13	1:B:631:MET:HG3	1.96	0.46
1:C:30:MET:HE3	1:C:633:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:ASN:HD22	1:C:687:ASN:H	1.59	0.46
1:D:44:TYR:HB3	5:D:2009:HOH:O	2.16	0.46
1:E:431:HIS:CD2	1:E:432:PRO:HD2	2.51	0.46
1:F:611:TYR:HB2	1:F:620:ALA:HB2	1.96	0.46
1:G:472:TRP:CE2	1:G:476:ARG:HD3	2.51	0.46
1:H:342:THR:OG1	1:H:388:PRO:HA	2.15	0.46
1:H:519:GLN:HE21	1:H:519:GLN:HB3	1.63	0.46
1:H:547:PRO:HB2	1:H:613:TYR:CD2	2.51	0.46
1:B:334:GLN:HA	5:B:2053:HOH:O	2.15	0.46
1:B:570:VAL:O	1:B:595:GLY:HA2	2.16	0.46
1:D:320:ASP:OD1	1:D:322:ASN:N	2.48	0.46
1:D:459:GLU:O	1:D:463:ARG:HG3	2.16	0.46
1:F:601:ASN:HB3	5:F:2040:HOH:O	2.14	0.46
1:H:454:ASP:OD2	1:H:513:ASN:HB3	2.16	0.46
1:B:153:PHE:CD1	1:B:159:SER:HB3	2.51	0.46
1:B:503:ASP:OD2	1:B:506:SER:OG	2.25	0.46
1:D:364:VAL:CG1	1:D:368:MET:HE3	2.44	0.46
1:D:420:TYR:O	1:D:424:ILE:HG12	2.16	0.46
1:E:60:THR:O	1:E:77:ARG:NH1	2.45	0.46
1:E:685:ASN:HD21	1:E:687:ASN:H	1.56	0.46
1:H:330:PRO:HB3	1:H:388:PRO:HB2	1.97	0.46
1:H:745:GLU:C	1:H:745:GLU:CD	2.84	0.46
1:A:91:ASP:OD1	1:A:92:TYR:N	2.45	0.46
1:C:611:TYR:HB2	1:C:620:ALA:HB2	1.97	0.46
1:F:29:LEU:HD23	1:F:45:PRO:HG3	1.97	0.46
1:F:754:LYS:O	1:F:755:GLU:HB3	2.16	0.46
1:A:602:GLN:N	1:A:603:PRO:CD	2.78	0.46
1:B:685:ASN:HD22	1:B:687:ASN:H	1.58	0.46
1:C:586:ILE:O	1:C:590:THR:HG23	2.15	0.46
1:D:533:GLU:OE2	3:D:801:SWA:C8	2.63	0.46
1:E:350:PHE:CD2	1:E:350:PHE:C	2.94	0.46
1:F:616:GLN:HG2	1:F:618:TRP:CH2	2.51	0.46
1:H:21:ASP:OD2	1:H:24:GLN:HG2	2.16	0.46
1:H:398:ASN:O	1:H:399:SER:C	2.57	0.46
1:A:153:PHE:CD1	1:A:159:SER:HB3	2.51	0.46
1:A:194:GLU:HB3	1:C:725:LYS:HG2	1.97	0.46
1:B:680:THR:C	1:B:681:LEU:HD23	2.41	0.46
1:D:354:PHE:N	1:D:355:PRO:CD	2.79	0.46
1:D:365:ASN:O	1:D:369:GLN:HG2	2.16	0.46
1:G:519:GLN:OE1	1:G:521:PRO:O	2.34	0.46
1:H:398:ASN:C	1:H:400:ALA:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LYS:N	1:A:485:LYS:CE	2.35	0.45
1:D:528:GLY:O	1:D:529:ASP:CB	2.62	0.45
1:E:419:LEU:HD12	1:E:419:LEU:O	2.17	0.45
1:F:21:ASP:OD1	1:F:23:THR:N	2.49	0.45
1:F:209:THR:O	1:F:209:THR:CG2	2.64	0.45
1:F:546:ASP:N	1:F:547:PRO:HD3	2.30	0.45
1:F:592[B]:MET:HG3	1:F:631:MET:HE1	1.97	0.45
1:H:442:TYR:CE1	1:H:443:GLU:CD	2.93	0.45
1:H:570:VAL:O	1:H:595:GLY:HA2	2.16	0.45
1:A:365:ASN:O	1:A:369:GLN:HG2	2.16	0.45
1:C:209:THR:O	1:C:209:THR:CG2	2.62	0.45
1:C:253:PHE:O	4:C:803:GOL:O1	2.13	0.45
1:F:316:PHE:CE2	1:F:330:PRO:HG3	2.52	0.45
1:F:483:ARG:HH21	1:F:487:GLU:CD	2.24	0.45
1:H:623:TRP:O	1:H:626:GLN:HB2	2.15	0.45
1:F:494:ARG:HA	1:F:497:ASN:ND2	2.31	0.45
1:G:147:VAL:CG2	1:G:148:LEU:N	2.78	0.45
1:G:177:GLU:H	1:G:177:GLU:CD	2.24	0.45
1:G:455:VAL:O	1:G:456:LYS:HB2	2.16	0.45
1:G:570:VAL:HG23	1:G:571:PRO:O	2.17	0.45
1:G:685:ASN:HD22	1:G:687:ASN:H	1.58	0.45
1:H:559:MET:HE3	1:H:559:MET:HB2	1.84	0.45
1:H:703:ILE:HD13	1:H:706:MET:HE2	1.98	0.45
1:H:717:TYR:C	1:H:718:LEU:HD23	2.42	0.45
1:A:583:ILE:HD12	1:A:585:GLU:HG2	1.98	0.45
1:B:592[B]:MET:CE	1:B:631:MET:HE3	2.27	0.45
1:D:165:ALA:O	1:D:166:PHE:HB2	2.16	0.45
1:E:240:ARG:NH1	1:E:240:ARG:HB2	2.32	0.45
1:F:354:PHE:CD2	1:F:402:ILE:HD12	2.52	0.45
1:F:612:ASP:OD2	1:F:671:MET:O	2.35	0.45
1:F:717:TYR:C	1:F:718:LEU:HD23	2.41	0.45
1:G:364:VAL:CG1	1:G:368:MET:HE3	2.45	0.45
1:G:526:LYS:O	1:G:535:ASN:HB3	2.17	0.45
1:H:360:MET:HE3	1:H:360:MET:HB3	1.80	0.45
1:A:483:ARG:HH21	1:A:487:GLU:CD	2.25	0.45
1:B:270:ASN:OD1	1:B:273:GLN:HG3	2.17	0.45
1:E:358:ASN:HD21	1:E:365:ASN:ND2	2.14	0.45
1:F:745:GLU:C	1:F:745:GLU:CD	2.85	0.45
1:H:748:MET:HE2	1:H:748:MET:N	2.32	0.45
1:B:403:LEU:HD22	1:B:419:LEU:CD1	2.45	0.45
1:B:685:ASN:HD21	1:B:687:ASN:H	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:ASN:HD22	1:C:735:ASN:HB3	1.81	0.45
1:D:284:GLN:HG2	5:D:2038:HOH:O	2.16	0.45
1:H:507:LYS:NZ	1:H:554:MET:O	2.38	0.45
1:A:29:LEU:HD23	1:A:45:PRO:HG3	1.98	0.45
1:A:503:ASP:C	1:A:503:ASP:OD1	2.59	0.45
1:D:397:ASN:HD22	1:D:439:ARG:NE	2.09	0.45
1:D:570:VAL:O	1:D:570:VAL:HG23	2.14	0.45
1:E:451:VAL:O	1:E:460:ASN:HB2	2.16	0.45
1:F:393:CYS:O	1:F:394:MET:HB2	2.17	0.45
1:G:329:SER:OG	1:G:378:GLU:OE1	2.28	0.45
1:G:330:PRO:HB3	1:G:388:PRO:HB2	1.97	0.45
1:H:610:LEU:HA	1:H:610:LEU:HD12	1.64	0.45
1:A:240:ARG:HB2	1:A:240:ARG:NH1	2.32	0.45
1:A:547:PRO:HB2	1:A:613:TYR:CD2	2.52	0.45
1:C:546:ASP:N	1:C:547:PRO:HD3	2.31	0.45
1:D:39:SER:HB3	1:D:588:GLU:OE2	2.17	0.45
1:D:101:VAL:HG13	1:D:156:ASN:ND2	2.32	0.45
1:D:257:GLU:HB2	5:D:2031:HOH:O	2.17	0.45
1:D:336:LEU:HB3	1:D:337:PRO:HD2	1.99	0.45
1:D:550:LEU:HD12	1:D:553:LEU:HD12	1.97	0.45
1:D:745:GLU:C	1:D:745:GLU:OE1	2.60	0.45
1:A:705:SER:OG	1:A:732[A]:ASP:OD2	2.30	0.45
1:B:177:GLU:H	1:B:177:GLU:CD	2.24	0.45
1:B:354:PHE:CD2	1:B:402:ILE:HD12	2.52	0.45
1:B:484:PRO:HB3	1:B:486:LYS:CE	2.47	0.45
1:A:703:ILE:HD13	1:A:706:MET:HE2	1.99	0.45
1:A:745:GLU:C	1:A:745:GLU:CD	2.84	0.45
1:B:90:ASN:HB3	1:B:189:SER:OG	2.17	0.45
1:F:175:ILE:O	1:F:175:ILE:HG22	2.17	0.45
1:F:417:LYS:O	1:F:421:GLU:HG3	2.16	0.45
1:G:745:GLU:C	1:G:745:GLU:CD	2.85	0.45
1:H:697:SER:OG	1:H:700:ASN:N	2.43	0.45
1:A:213:THR:HG23	1:A:223:VAL:O	2.17	0.44
1:E:177:GLU:H	1:E:177:GLU:CD	2.25	0.44
1:E:295:ASN:OD1	1:E:297:ASP:HB2	2.17	0.44
1:F:570:VAL:O	1:F:595:GLY:HA2	2.16	0.44
1:G:570:VAL:O	1:G:595:GLY:HA2	2.17	0.44
1:H:393:CYS:O	1:H:394:MET:HB2	2.17	0.44
1:H:458:ASN:O	1:H:459:GLU:HB2	2.16	0.44
1:B:350:PHE:CD2	1:B:350:PHE:C	2.95	0.44
1:D:288:LYS:NZ	4:D:804:GOL:H31	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:VAL:O	1:D:595:GLY:HA2	2.16	0.44
1:G:481:LEU:N	1:G:481:LEU:CD1	2.79	0.44
1:B:459:GLU:CG	1:B:532:THR:HG22	2.46	0.44
1:C:510:ARG:NH2	1:C:519:GLN:O	2.37	0.44
1:C:624:LEU:HD12	1:C:624:LEU:HA	1.84	0.44
1:D:354:PHE:CD2	1:D:402:ILE:HD12	2.52	0.44
1:E:663:CYS:O	1:E:666:THR:HG23	2.18	0.44
1:F:90:ASN:HB3	1:F:189:SER:OG	2.17	0.44
1:F:342:THR:OG1	1:F:388:PRO:HA	2.17	0.44
1:H:332:ASN:C	1:H:332:ASN:OD1	2.60	0.44
1:H:602:GLN:N	1:H:603:PRO:CD	2.80	0.44
1:A:57:THR:OG1	1:A:58:PRO:HD2	2.17	0.44
3:C:801:SWA:HC52	5:C:2061:HOH:O	2.17	0.44
1:D:213:THR:HG23	1:D:223:VAL:O	2.16	0.44
1:F:541:TRP:CH2	1:F:564:MET:HG2	2.53	0.44
1:G:472:TRP:CZ2	1:G:476:ARG:CD	3.00	0.44
1:G:477:LEU:HG	1:G:481:LEU:HD22	1.99	0.44
1:A:59:GLN:HE21	1:A:80:LYS:HB2	1.82	0.44
1:B:611:TYR:HB2	1:B:620:ALA:HB2	1.99	0.44
1:C:703:ILE:HD13	1:C:706:MET:HE2	1.99	0.44
1:D:105:VAL:O	1:D:105:VAL:HG23	2.18	0.44
1:D:330:PRO:HB3	1:D:388:PRO:HB2	1.98	0.44
1:D:485:LYS:HB2	1:D:485:LYS:HE3	1.75	0.44
1:D:703:ILE:HD13	1:D:706:MET:HE2	1.99	0.44
1:E:26:VAL:HG11	1:E:124:PRO:HG3	1.98	0.44
1:E:145:ARG:NH2	1:E:317:TYR:O	2.33	0.44
1:G:39:SER:HB3	1:G:588:GLU:OE2	2.18	0.44
1:G:481:LEU:N	1:G:481:LEU:HD13	2.33	0.44
1:B:451:VAL:O	1:B:460:ASN:HB2	2.16	0.44
1:C:627:VAL:HG13	1:C:631:MET:HG3	1.98	0.44
1:E:459:GLU:CG	1:E:532:THR:HG22	2.47	0.44
1:A:472:TRP:CE2	1:A:476:ARG:HD3	2.53	0.44
1:C:486:LYS:HA	1:C:486:LYS:HD3	1.25	0.44
1:F:62:LYS:HE3	1:F:109:GLU:OE2	2.18	0.44
1:H:339:TYR:CE1	1:H:367:GLU:CD	2.96	0.44
1:H:343:ASP:HA	1:H:386:ALA:O	2.18	0.44
1:H:459:GLU:HA	1:H:530:ALA:O	2.18	0.44
1:B:750:TYR:CE1	1:B:755:GLU:OE2	2.70	0.44
1:C:592[B]:MET:CG	1:C:631:MET:HE1	2.48	0.44
1:E:428:GLU:HA	1:E:442:TYR:CD2	2.53	0.44
1:E:593:ASN:HB2	1:F:130:TYR:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:604:ILE:O	1:E:604:ILE:HG23	2.17	0.44
1:G:53:MET:CE	1:G:145:ARG:HG2	2.39	0.44
1:H:689:LEU:C	1:H:689:LEU:HD13	2.42	0.44
1:B:405:ASP:O	1:B:409:LYS:HG3	2.17	0.44
1:G:517:THR:H	1:G:517:THR:HG1	1.42	0.44
1:B:550:LEU:HD12	1:B:553:LEU:HD12	2.00	0.43
1:C:623:TRP:O	1:C:626:GLN:HB2	2.18	0.43
1:D:30:MET:HE3	1:D:633:THR:O	2.17	0.43
1:D:327:HIS:ND1	1:D:338:GLY:O	2.46	0.43
1:D:481:LEU:N	1:D:481:LEU:CD1	2.81	0.43
1:F:361:TYR:N	1:F:362:PRO:CD	2.81	0.43
1:G:143:THR:OG1	1:G:265:GLU:OE1	2.21	0.43
1:G:145:ARG:HD2	1:G:265:GLU:OE2	2.17	0.43
1:G:315:LYS:HE2	1:G:317:TYR:OH	2.17	0.43
1:G:494:ARG:HA	1:G:497:ASN:ND2	2.32	0.43
1:A:354:PHE:N	1:A:355:PRO:CD	2.81	0.43
1:B:503:ASP:C	1:B:503:ASP:OD1	2.62	0.43
1:E:327:HIS:ND1	1:E:338:GLY:O	2.47	0.43
1:E:461:ALA:HB3	1:E:530:ALA:O	2.17	0.43
1:E:586:ILE:O	1:E:590:THR:HG23	2.19	0.43
1:F:240:ARG:HB2	1:F:240:ARG:NH1	2.33	0.43
1:H:431:HIS:HD2	1:H:433:GLU:N	2.11	0.43
1:H:609:TYR:CE2	1:H:624:LEU:HD21	2.53	0.43
1:A:331:TYR:CE2	1:A:375:THR:HG23	2.52	0.43
1:B:745:GLU:C	1:B:745:GLU:CD	2.86	0.43
1:C:319:LEU:HD12	1:C:319:LEU:HA	1.84	0.43
1:C:459:GLU:CG	1:C:532:THR:HG22	2.46	0.43
1:E:528:GLY:O	1:E:529:ASP:CB	2.66	0.43
1:F:209:THR:O	1:F:209:THR:HG22	2.17	0.43
1:F:477:LEU:HG	1:F:481:LEU:HD22	2.00	0.43
1:F:502:PHE:CD2	1:F:502:PHE:C	2.97	0.43
1:G:426:GLY:O	1:G:439:ARG:HG3	2.18	0.43
1:G:586:ILE:O	1:G:590:THR:HG23	2.19	0.43
1:G:602:GLN:N	1:G:603:PRO:CD	2.80	0.43
1:A:481:LEU:HD13	1:A:481:LEU:N	2.34	0.43
1:C:332:ASN:C	1:C:332:ASN:OD1	2.61	0.43
1:C:519:GLN:OE1	1:C:521:PRO:O	2.36	0.43
1:C:745:GLU:C	1:C:745:GLU:CD	2.85	0.43
1:E:354:PHE:CD2	1:E:402:ILE:HD12	2.53	0.43
1:E:477:LEU:HG	1:E:481:LEU:HD22	1.99	0.43
1:E:616:GLN:HG2	1:E:618:TRP:CH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:THR:HB	1:G:237:PHE:HA	2.00	0.43
1:H:419:LEU:HD12	1:H:419:LEU:O	2.18	0.43
1:H:484:PRO:O	1:H:488:ILE:CG1	2.65	0.43
1:B:22:TRP:N	1:B:283:ASN:HD21	2.13	0.43
1:C:175:ILE:O	1:C:175:ILE:HG22	2.18	0.43
1:D:609:TYR:CE2	1:D:624:LEU:HD21	2.53	0.43
1:E:375:THR:O	1:E:379:SER:OG	2.23	0.43
1:E:475:TYR:CD2	1:E:492:ALA:HB2	2.54	0.43
1:G:144:GLU:OE2	1:G:315:LYS:NZ	2.37	0.43
1:G:553:LEU:HD22	1:G:553:LEU:N	2.27	0.43
1:D:754:LYS:O	1:D:755:GLU:C	2.62	0.43
1:E:570:VAL:HG23	1:E:571:PRO:O	2.19	0.43
1:F:517:THR:H	1:F:517:THR:HG1	1.54	0.43
1:F:602:GLN:N	1:F:603:PRO:CD	2.82	0.43
1:F:610:LEU:HD12	1:F:610:LEU:HA	1.68	0.43
1:H:560:PHE:CZ	1:H:564:MET:HE3	2.53	0.43
1:H:736:ARG:NH1	1:H:736:ARG:HB2	2.21	0.43
1:A:533:GLU:OE2	3:A:801:SWA:HC8	2.19	0.43
1:A:623:TRP:O	1:A:626:GLN:HB2	2.18	0.43
1:B:431:HIS:HA	1:B:432:PRO:HD3	1.85	0.43
1:D:453:TYR:CE1	1:D:519:GLN:HG3	2.53	0.43
1:E:316:PHE:CE2	1:E:330:PRO:HG3	2.54	0.43
1:E:550:LEU:CA	1:E:553:LEU:HD12	2.36	0.43
1:G:510:ARG:NH2	1:G:519:GLN:O	2.38	0.43
1:H:331:TYR:CZ	1:H:375:THR:CG2	2.97	0.43
1:A:35:THR:HA	5:A:2003:HOH:O	2.18	0.43
1:A:172:ILE:HG22	1:A:226:GLN:HB2	2.00	0.43
1:A:503:ASP:CG	1:A:506:SER:HG	2.25	0.43
1:B:519:GLN:HG2	1:B:520:SER:N	2.34	0.43
1:C:750:TYR:CD2	1:C:750:TYR:C	2.96	0.43
1:E:494:ARG:O	1:E:497:ASN:ND2	2.52	0.43
1:E:501:LEU:HA	1:E:501:LEU:HD23	1.76	0.43
1:A:216:ASN:HD22	1:A:216:ASN:N	2.16	0.43
1:A:529:ASP:HB3	1:A:530:ALA:H	1.57	0.43
1:A:570:VAL:HG23	1:A:571:PRO:O	2.19	0.43
1:B:612:ASP:OD2	1:B:671:MET:O	2.37	0.43
1:B:616:GLN:HG2	1:B:618:TRP:CH2	2.53	0.43
1:C:240:ARG:NH1	1:C:240:ARG:HB2	2.34	0.43
1:D:671:MET:HG2	1:D:706:MET:HE1	2.00	0.43
1:G:199:TYR:O	1:G:251:SER:HA	2.19	0.43
1:H:397:ASN:HD22	1:H:439:ARG:NE	2.04	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ASP:OD2	1:A:506:SER:OG	2.30	0.43
1:E:481:LEU:N	1:E:481:LEU:CD1	2.79	0.43
1:G:529:ASP:HB3	1:G:530:ALA:H	1.44	0.43
1:H:431:HIS:HB3	1:H:434:VAL:O	2.19	0.43
1:H:498:TYR:CD2	1:H:498:TYR:C	2.97	0.43
1:H:616:GLN:HG2	1:H:618:TRP:CZ2	2.53	0.43
1:H:632:TYR:C	1:H:633:THR:HG23	2.43	0.43
1:A:177:GLU:CD	1:A:177:GLU:H	2.27	0.42
1:A:252:SER:HG	1:A:318:GLU:CD	2.10	0.42
1:A:340:MET:HE2	1:A:340:MET:HB2	1.85	0.42
1:B:26:VAL:HG11	1:B:124:PRO:HG3	2.01	0.42
1:B:29:LEU:HD23	1:B:45:PRO:HG3	2.01	0.42
1:B:392:GLY:HA2	1:B:436:SER:OG	2.18	0.42
1:B:553:LEU:H	1:B:553:LEU:HG	1.49	0.42
1:D:528:GLY:O	1:D:529:ASP:HB3	2.19	0.42
1:F:532:THR:O	1:F:532:THR:OG1	2.35	0.42
1:G:612:ASP:OD2	1:G:671:MET:O	2.37	0.42
1:H:141:THR:O	1:H:147:VAL:CG2	2.67	0.42
1:A:481:LEU:N	1:A:481:LEU:CD1	2.81	0.42
1:C:616:GLN:HG2	1:C:618:TRP:CH2	2.54	0.42
1:C:616:GLN:HG2	1:C:618:TRP:CZ2	2.53	0.42
1:D:523:SER:HB2	1:D:526:LYS:HB2	2.01	0.42
1:E:431:HIS:HA	1:E:432:PRO:HD3	1.88	0.42
1:F:483:ARG:HB3	1:F:484:PRO:HD2	2.00	0.42
1:F:519:GLN:OE1	1:F:521:PRO:O	2.37	0.42
1:F:604:ILE:O	1:F:604:ILE:HG23	2.19	0.42
1:A:293:GLY:HA3	1:A:677:LYS:HB2	2.02	0.42
1:A:503:ASP:CG	1:A:506:SER:OG	2.61	0.42
1:B:165:ALA:O	1:B:166:PHE:HB2	2.19	0.42
1:B:610:LEU:HA	1:B:610:LEU:HD12	1.68	0.42
1:C:22:TRP:N	1:C:283:ASN:HD21	2.17	0.42
1:C:167:ASP:O	1:C:168:LYS:HB2	2.20	0.42
1:C:176:PRO:HD2	1:C:177:GLU:OE1	2.19	0.42
1:E:575:ASP:C	1:E:575:ASP:OD1	2.62	0.42
1:F:426:GLY:O	1:F:439:ARG:HG3	2.19	0.42
1:F:472:TRP:CZ2	1:F:476:ARG:CD	3.01	0.42
1:G:523:SER:HB2	1:G:526:LYS:HB2	2.00	0.42
1:H:59:GLN:HE21	1:H:80:LYS:HB2	1.83	0.42
1:H:365:ASN:O	1:H:369:GLN:N	2.42	0.42
1:H:417:LYS:NZ	1:H:421:GLU:OE2	2.30	0.42
1:A:268:LYS:HD3	1:A:268:LYS:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LYS:HD2	1:A:456:LYS:HA	1.57	0.42
1:A:624:LEU:HD12	1:A:624:LEU:HA	1.88	0.42
1:B:507:LYS:NZ	1:B:559[B]:MET:CE	2.82	0.42
1:D:507:LYS:CE	1:D:559:MET:HE2	2.45	0.42
1:D:602:GLN:N	1:D:603:PRO:CD	2.82	0.42
1:E:431:HIS:HB3	1:E:434:VAL:O	2.20	0.42
1:E:481:LEU:N	1:E:481:LEU:HD13	2.35	0.42
1:E:502:PHE:C	1:E:502:PHE:CD2	2.97	0.42
1:E:507:LYS:O	1:E:554:MET:HE2	2.18	0.42
1:H:448:LEU:N	1:H:448:LEU:CD2	2.79	0.42
1:B:240:ARG:NH1	1:B:240:ARG:HB2	2.35	0.42
1:B:327:HIS:ND1	1:B:338:GLY:O	2.51	0.42
1:D:331:TYR:CZ	1:D:375:THR:HG23	2.53	0.42
1:D:481:LEU:N	1:D:481:LEU:HD13	2.35	0.42
1:D:486:LYS:HB2	5:D:2073:HOH:O	2.18	0.42
1:E:602:GLN:NE2	1:E:644:ASP:OD2	2.52	0.42
1:F:592[A]:MET:HE2	1:F:640:CYS:HB2	2.01	0.42
1:H:364:VAL:HG12	1:H:368:MET:HE3	2.01	0.42
1:H:497:ASN:HA	1:H:500:ASN:HD21	1.82	0.42
1:H:616:GLN:HG2	1:H:618:TRP:CH2	2.54	0.42
1:A:616:GLN:HG2	1:A:618:TRP:CH2	2.55	0.42
1:C:62:LYS:HE3	1:C:109:GLU:OE2	2.19	0.42
1:C:431:HIS:HA	1:C:432:PRO:HD3	1.87	0.42
1:D:26:VAL:HG11	1:D:124:PRO:HG3	2.00	0.42
1:E:627:VAL:HG13	1:E:631:MET:HG3	2.02	0.42
1:F:59:GLN:HE21	1:F:80:LYS:HB2	1.84	0.42
1:G:458:ASN:O	1:G:459:GLU:HB2	2.19	0.42
1:H:365:ASN:HA	1:H:368:MET:HB2	2.01	0.42
1:H:497:ASN:CA	1:H:500:ASN:ND2	2.82	0.42
1:A:416:ILE:O	1:A:416:ILE:HG22	2.19	0.42
1:B:275:ALA:CB	4:B:803:GOL:H31	2.50	0.42
1:B:700:ASN:HD22	1:B:735:ASN:HB3	1.85	0.42
1:C:523:SER:HB2	1:C:526:LYS:HB2	2.01	0.42
1:D:167:ASP:O	1:D:168:LYS:CB	2.61	0.42
1:D:519:GLN:HE21	1:D:519:GLN:HB3	1.60	0.42
1:E:168:LYS:HD3	1:E:168:LYS:HA	1.80	0.42
1:E:354:PHE:N	1:E:355:PRO:CD	2.82	0.42
1:G:496:MET:HE2	1:G:752:PHE:CE2	2.54	0.42
1:H:213:THR:HG23	1:H:223:VAL:O	2.20	0.42
1:H:475:TYR:CE2	1:H:479:LYS:HD3	2.55	0.42
1:B:168:LYS:HA	1:B:168:LYS:HD3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:THR:OG1	1:B:388:PRO:HA	2.20	0.42
3:C:801:SWA:HC91	5:C:2061:HOH:O	2.19	0.42
1:D:216:ASN:HD21	1:D:229:ASP:HB3	1.84	0.42
1:D:426:GLY:O	1:D:439:ARG:HG3	2.19	0.42
1:D:606:HIS:HB3	5:D:2096:HOH:O	2.20	0.42
1:F:459:GLU:O	1:F:463:ARG:HG3	2.20	0.42
1:F:602:GLN:NE2	1:F:644:ASP:OD2	2.53	0.42
1:G:252:SER:HG	1:G:318:GLU:CD	2.13	0.42
1:H:453:TYR:CE1	1:H:519:GLN:HG3	2.55	0.42
1:H:612:ASP:OD2	1:H:671:MET:O	2.38	0.42
1:A:622:TYR:CD2	1:A:622:TYR:C	2.98	0.42
1:B:459:GLU:HG2	1:B:531:PHE:O	2.20	0.42
1:D:663:CYS:O	1:D:666:THR:HG23	2.20	0.42
1:B:194:GLU:HG2	5:B:2026:HOH:O	2.19	0.42
1:B:385:TRP:CD1	1:B:393:CYS:HB3	2.55	0.42
1:D:22:TRP:N	1:D:283:ASN:HD21	2.08	0.42
1:F:519:GLN:HE21	1:F:519:GLN:HB3	1.61	0.42
1:G:168:LYS:HD3	1:G:168:LYS:HA	1.82	0.42
1:H:358:ASN:ND2	1:H:365:ASN:HD22	2.17	0.42
1:A:452:PRO:HB2	1:A:455:VAL:HG13	2.02	0.41
1:B:706:MET:CE	1:B:741:ARG:NH2	2.54	0.41
1:C:177:GLU:CD	1:C:177:GLU:H	2.27	0.41
1:C:316:PHE:CE2	1:C:330:PRO:HG3	2.55	0.41
1:D:583:ILE:HD12	1:D:585:GLU:HG2	2.02	0.41
1:F:592[B]:MET:SD	1:F:631:MET:CE	2.96	0.41
1:G:559:MET:HE2	1:G:559:MET:HB3	1.87	0.41
1:H:354:PHE:N	1:H:355:PRO:CD	2.83	0.41
1:A:209:THR:HB	1:A:237:PHE:HA	2.01	0.41
1:B:472:TRP:CZ2	1:B:476:ARG:CD	3.03	0.41
1:B:623:TRP:O	1:B:626:GLN:HB2	2.20	0.41
1:D:361:TYR:N	1:D:362:PRO:CD	2.82	0.41
1:E:735:ASN:OD1	1:E:736:ARG:HG3	2.20	0.41
1:G:407:TYR:CZ	1:G:412:LYS:CD	2.96	0.41
1:H:22:TRP:N	1:H:283:ASN:HD21	2.17	0.41
1:H:186:THR:O	1:H:187:ARG:C	2.62	0.41
1:H:477:LEU:O	1:H:480:GLU:HB3	2.20	0.41
1:H:497:ASN:O	1:H:499:LYS:N	2.53	0.41
1:A:84:GLN:HG3	1:A:90:ASN:C	2.45	0.41
1:B:373:ILE:HG23	1:B:373:ILE:HD12	1.82	0.41
1:B:602:GLN:N	1:B:603:PRO:CD	2.83	0.41
1:D:59:GLN:HE21	1:D:80:LYS:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:THR:HB	1:D:237:PHE:HA	2.02	0.41
1:D:375:THR:CG2	1:D:383:PRO:HD3	2.48	0.41
1:D:553:LEU:HG	1:D:553:LEU:H	1.55	0.41
1:D:721:GLU:H	1:D:721:GLU:CD	2.28	0.41
1:G:431:HIS:HB3	1:G:434:VAL:O	2.20	0.41
1:H:167:ASP:O	1:H:168:LYS:HB2	2.20	0.41
1:H:177:GLU:CD	1:H:177:GLU:H	2.28	0.41
1:H:553:LEU:H	1:H:553:LEU:HG	1.60	0.41
1:C:352:CYS:C	1:C:355:PRO:HD2	2.45	0.41
1:D:709:ASN:ND2	1:D:728:THR:H	2.18	0.41
1:E:319:LEU:HD12	1:E:319:LEU:HA	1.84	0.41
1:F:523:SER:HB2	1:F:526:LYS:HB2	2.02	0.41
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.80	0.41
1:D:199:TYR:O	1:D:251:SER:HA	2.20	0.41
1:E:472:TRP:CE2	1:E:476:ARG:HD3	2.55	0.41
1:E:592:MET:HE1	1:E:600:GLY:H	1.85	0.41
1:F:706:MET:HE3	1:F:741:ARG:CZ	2.41	0.41
1:H:90:ASN:HB3	1:H:189:SER:OG	2.20	0.41
1:H:431:HIS:HA	1:H:432:PRO:HD3	1.87	0.41
1:H:459:GLU:CG	1:H:532:THR:HG22	2.50	0.41
1:H:498:TYR:OH	1:H:546:ASP:OD2	2.35	0.41
1:B:63:MET:HG3	1:B:166:PHE:CE2	2.54	0.41
1:B:484:PRO:HB3	1:B:486:LYS:HZ2	1.86	0.41
1:B:624:LEU:HD12	1:B:624:LEU:HA	1.85	0.41
1:C:105:VAL:O	1:C:105:VAL:HG23	2.18	0.41
1:C:268:LYS:HD3	1:C:268:LYS:HA	1.84	0.41
1:C:455:VAL:O	1:C:456:LYS:HB2	2.19	0.41
1:D:487:GLU:HG3	5:D:2074:HOH:O	2.19	0.41
1:D:610:LEU:HD12	1:D:610:LEU:HA	1.68	0.41
1:A:524:PRO:HD2	5:A:2081:HOH:O	2.19	0.41
1:A:546:ASP:N	1:A:547:PRO:HD3	2.36	0.41
1:B:332:ASN:OD1	1:B:332:ASN:C	2.63	0.41
1:B:519:GLN:OE1	1:B:521:PRO:O	2.38	0.41
1:D:88:TRP:HB2	3:D:801:SWA:HC62	2.01	0.41
1:D:352:CYS:C	1:D:355:PRO:HD2	2.45	0.41
1:D:623:TRP:O	1:D:626:GLN:HB2	2.20	0.41
1:E:448:LEU:HD22	1:E:448:LEU:N	2.36	0.41
1:F:168:LYS:HA	1:F:168:LYS:HD3	1.81	0.41
1:G:107:ASP:OD1	1:G:109:GLU:N	2.41	0.41
1:G:360:MET:HE3	1:G:360:MET:HB3	1.90	0.41
1:H:293:GLY:HA3	1:H:677:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:420:TYR:O	1:H:424:ILE:HG12	2.21	0.41
1:A:483:ARG:HB3	1:A:487:GLU:OE2	2.21	0.41
1:B:319:LEU:HD12	1:B:319:LEU:HA	1.84	0.41
1:B:458:ASN:O	1:B:459:GLU:HB2	2.20	0.41
1:B:754:LYS:O	1:B:755:GLU:CG	2.69	0.41
1:C:420:TYR:O	1:C:424:ILE:HG12	2.21	0.41
1:D:505:GLU:HG2	1:D:506:SER:H	1.83	0.41
1:D:547:PRO:HB2	1:D:613:TYR:CD2	2.56	0.41
3:D:801:SWA:HC52	5:D:2094:HOH:O	2.19	0.41
1:F:216:ASN:CB	5:F:2021:HOH:O	2.54	0.41
1:G:554:MET:O	1:G:559:MET:HE2	2.21	0.41
1:A:354:PHE:CD2	1:A:402:ILE:HD12	2.56	0.41
1:B:142:PRO:HA	1:B:147:VAL:HA	2.03	0.41
1:C:448:LEU:HD22	1:C:448:LEU:N	2.36	0.41
1:C:549:GLY:O	1:C:553:LEU:HG	2.20	0.41
1:D:453:TYR:N	1:D:512:ARG:O	2.40	0.41
1:D:503:ASP:OD1	1:D:505:GLU:N	2.54	0.41
1:E:523:SER:HB2	1:E:526:LYS:HB2	2.02	0.41
1:F:30:MET:HE3	1:F:633:THR:O	2.19	0.41
1:F:481:LEU:HA	1:F:481:LEU:HD12	1.89	0.41
1:G:84:GLN:HG3	1:G:90:ASN:C	2.46	0.41
1:G:268:LYS:HA	1:G:268:LYS:HD3	1.84	0.41
1:H:199:TYR:O	1:H:251:SER:HA	2.21	0.41
1:H:452:PRO:HB2	1:H:455:VAL:HG22	2.01	0.41
1:H:671:MET:HG2	1:H:706:MET:HE1	2.02	0.41
1:A:193:PRO:HB3	5:A:2058:HOH:O	2.21	0.41
1:A:689:LEU:HD22	1:A:690:VAL:N	2.36	0.41
1:B:80:LYS:HE3	1:B:94:GLN:HB2	2.02	0.41
1:D:255:SER:HB2	5:D:2030:HOH:O	2.21	0.41
1:E:475:TYR:OH	1:E:755:GLU:OE1	2.38	0.41
1:E:494:ARG:HA	1:E:497:ASN:ND2	2.36	0.41
1:F:354:PHE:N	1:F:355:PRO:CD	2.84	0.41
1:G:419:LEU:HD12	1:G:419:LEU:C	2.46	0.41
1:G:456:LYS:HA	1:G:456:LYS:HD2	1.73	0.41
1:G:547:PRO:CB	1:G:613:TYR:CD2	3.04	0.41
1:H:541:TRP:CH2	1:H:564:MET:HG2	2.56	0.41
1:H:627:VAL:HG13	1:H:631:MET:HG3	2.03	0.41
1:A:431:HIS:HB3	1:A:434:VAL:O	2.21	0.40
1:B:622:TYR:CD2	1:B:622:TYR:C	2.99	0.40
1:B:681:LEU:O	1:B:688:SER:HA	2.21	0.40
1:D:238:LYS:HE3	1:D:238:LYS:HB3	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:612:ASP:OD2	1:E:671:MET:O	2.39	0.40
1:G:319:LEU:HD12	1:G:319:LEU:HA	1.80	0.40
1:G:327:HIS:ND1	1:G:338:GLY:O	2.51	0.40
1:G:394:MET:HA	1:G:394:MET:HE3	2.03	0.40
1:G:543:VAL:HG12	1:G:543:VAL:O	2.21	0.40
1:A:390:HIS:H	4:A:804:GOL:H2	1.86	0.40
1:A:431:HIS:HD2	1:A:434:VAL:H	1.65	0.40
1:A:586:ILE:O	1:A:590:THR:HG23	2.21	0.40
1:B:210:TYR:CD1	1:B:210:TYR:C	2.99	0.40
1:D:316:PHE:CE2	1:D:330:PRO:HG3	2.56	0.40
1:D:350:PHE:CD2	1:D:350:PHE:C	2.98	0.40
1:D:385:TRP:CD1	1:D:393:CYS:HB3	2.56	0.40
1:E:353:LEU:C	1:E:353:LEU:HD13	2.46	0.40
1:E:361:TYR:N	1:E:362:PRO:HD3	2.37	0.40
1:F:503:ASP:OD1	1:F:503:ASP:C	2.64	0.40
1:G:549:GLY:O	1:G:553:LEU:CD1	2.69	0.40
1:H:528:GLY:HA2	1:H:531:PHE:O	2.21	0.40
1:H:586:ILE:O	1:H:590:THR:HG23	2.21	0.40
1:A:72:THR:HG21	1:B:72:THR:HG21	2.03	0.40
1:A:681:LEU:HD23	1:A:681:LEU:N	2.35	0.40
1:B:507:LYS:HZ2	1:B:559[B]:MET:HE2	1.85	0.40
1:C:494:ARG:O	1:C:497:ASN:ND2	2.55	0.40
1:D:612:ASP:OD2	1:D:671:MET:O	2.39	0.40
1:D:624:LEU:HD12	1:D:624:LEU:HA	1.91	0.40
1:F:295:ASN:OD1	1:F:297:ASP:HB2	2.22	0.40
1:G:210:TYR:CD1	1:G:210:TYR:C	2.99	0.40
1:H:29:LEU:HD23	1:H:45:PRO:HG3	2.03	0.40
1:H:176:PRO:HD2	1:H:177:GLU:OE1	2.22	0.40
1:H:447:LYS:CG	1:H:448:LEU:HD22	2.51	0.40
1:A:168:LYS:HD3	1:A:168:LYS:HA	1.83	0.40
1:C:90:ASN:HB3	1:C:189:SER:OG	2.21	0.40
1:C:354:PHE:N	1:C:355:PRO:CD	2.85	0.40
1:D:188:ASN:ND2	1:D:190:GLY:H	2.12	0.40
1:D:443:GLU:H	1:D:443:GLU:CD	2.24	0.40
1:E:624:LEU:HD12	1:E:624:LEU:HA	1.86	0.40
1:F:63:MET:HB3	5:F:2009:HOH:O	2.21	0.40
1:F:176:PRO:HD2	1:F:177:GLU:OE1	2.21	0.40
1:G:459:GLU:CG	1:G:532:THR:HG22	2.51	0.40
1:G:528:GLY:O	1:G:529:ASP:CB	2.69	0.40
1:H:142:PRO:HA	1:H:147:VAL:HA	2.04	0.40
1:H:268:LYS:HA	1:H:268:LYS:HD3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:TRP:CZ2	1:A:476:ARG:CD	3.05	0.40
1:B:283:ASN:HD22	1:B:283:ASN:HA	1.77	0.40
1:C:481:LEU:N	1:C:481:LEU:CD1	2.84	0.40
1:C:519:GLN:HE21	1:C:519:GLN:HB3	1.70	0.40
1:D:186:THR:O	1:D:187:ARG:C	2.64	0.40
1:D:431:HIS:HB3	1:D:434:VAL:O	2.22	0.40
1:D:494:ARG:HA	1:D:497:ASN:ND2	2.37	0.40
1:E:186:THR:O	1:E:187:ARG:C	2.62	0.40
1:E:528:GLY:O	1:E:529:ASP:HB3	2.22	0.40
1:F:134:HIS:O	1:F:135:ASP:HB3	2.22	0.40
1:F:177:GLU:CD	1:F:177:GLU:H	2.28	0.40
1:F:415:ASP:CG	1:F:418:THR:HG1	2.16	0.40
1:F:452:PRO:HB2	1:F:455:VAL:HG13	2.04	0.40
1:H:721:GLU:N	1:H:721:GLU:CD	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/744 (99%)	713 (97%)	22 (3%)	2 (0%)	36	66
1	B	739/744 (99%)	711 (96%)	26 (4%)	2 (0%)	36	66
1	C	737/744 (99%)	712 (97%)	23 (3%)	2 (0%)	36	66
1	D	738/744 (99%)	710 (96%)	26 (4%)	2 (0%)	36	66
1	E	736/744 (99%)	711 (97%)	23 (3%)	2 (0%)	36	66
1	F	735/744 (99%)	709 (96%)	23 (3%)	3 (0%)	30	60
1	G	734/744 (99%)	707 (96%)	25 (3%)	2 (0%)	36	66
1	H	734/744 (99%)	707 (96%)	25 (3%)	2 (0%)	36	66
All	All	5890/5952 (99%)	5680 (96%)	193 (3%)	17 (0%)	36	66

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	521	PRO
1	C	521	PRO
1	F	521	PRO
1	G	521	PRO
1	A	521	PRO
1	D	521	PRO
1	E	521	PRO
1	C	313	PRO
1	D	313	PRO
1	E	313	PRO
1	F	313	PRO
1	B	313	PRO
1	G	313	PRO
1	H	313	PRO
1	F	529	ASP
1	H	142	PRO
1	A	313	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	636/643 (99%)	601 (94%)	35 (6%)	19	51
1	B	640/643 (100%)	605 (94%)	35 (6%)	19	51
1	C	636/643 (99%)	603 (95%)	33 (5%)	21	53
1	D	636/643 (99%)	599 (94%)	37 (6%)	18	49
1	E	631/643 (98%)	597 (95%)	34 (5%)	20	51
1	F	631/643 (98%)	593 (94%)	38 (6%)	17	47
1	G	626/643 (97%)	595 (95%)	31 (5%)	22	54
1	H	618/643 (96%)	583 (94%)	35 (6%)	18	49
All	All	5054/5144 (98%)	4776 (94%)	278 (6%)	19	51

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ARG
1	A	101	VAL
1	A	177	GLU
1	A	206	LYS
1	A	209	THR
1	A	220	GLN
1	A	237	PHE
1	A	284	GLN
1	A	319	LEU
1	A	363	SER
1	A	385	TRP
1	A	456	LYS
1	A	479	LYS
1	A	481	LEU
1	A	485	LYS
1	A	486	LYS
1	A	504	LYS
1	A	505	GLU
1	A	517	THR
1	A	519	GLN
1	A	553	LEU
1	A	559	MET
1	A	564	MET
1	A	573	ILE
1	A	585	GLU
1	A	610	LEU
1	A	624	LEU
1	A	685	ASN
1	A	689	LEU
1	A	692	ASP
1	A	714	THR
1	A	730	LYS
1	A	732[A]	ASP
1	A	732[B]	ASP
1	A	739	LEU
1	B	20	LYS
1	B	77	ARG
1	B	101	VAL
1	B	177	GLU
1	B	206	LYS
1	B	220	GLN
1	B	237	PHE
1	B	284	GLN

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Mol	Chain	Res	Type
1	B	319	LEU
1	B	355	PRO
1	B	363	SER
1	B	385	TRP
1	B	456	LYS
1	B	479	LYS
1	B	481	LEU
1	B	486	LYS
1	B	506	SER
1	B	517	THR
1	B	519	GLN
1	B	553	LEU
1	B	559[A]	MET
1	B	559[B]	MET
1	B	564	MET
1	B	573	ILE
1	B	585	GLU
1	B	604	ILE
1	B	610	LEU
1	B	624	LEU
1	B	685	ASN
1	B	689	LEU
1	B	692	ASP
1	B	714	THR
1	B	730	LYS
1	B	736	ARG
1	B	739	LEU
1	C	77	ARG
1	C	101	VAL
1	C	177	GLU
1	C	220	GLN
1	C	237	PHE
1	C	284	GLN
1	C	319	LEU
1	C	363	SER
1	C	385	TRP
1	C	479	LYS
1	C	481	LEU
1	C	486	LYS
1	C	504	LYS
1	C	506	SER
1	C	517	THR

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Mol	Chain	Res	Type
1	C	519	GLN
1	C	553	LEU
1	C	564	MET
1	C	570	VAL
1	C	573	ILE
1	C	577	SER
1	C	585	GLU
1	C	596	ASN
1	C	610	LEU
1	C	624	LEU
1	C	685	ASN
1	C	689	LEU
1	C	692	ASP
1	C	714	THR
1	C	730	LYS
1	C	739	LEU
1	C	753	SER
1	C	756	LEU
1	D	21	ASP
1	D	77	ARG
1	D	101	VAL
1	D	177	GLU
1	D	209	THR
1	D	220	GLN
1	D	237	PHE
1	D	284	GLN
1	D	319	LEU
1	D	363	SER
1	D	385	TRP
1	D	433	GLU
1	D	443	GLU
1	D	479	LYS
1	D	481	LEU
1	D	485	LYS
1	D	504	LYS
1	D	505	GLU
1	D	506	SER
1	D	517	THR
1	D	519	GLN
1	D	553	LEU
1	D	564	MET
1	D	570	VAL

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Mol	Chain	Res	Type
1	D	573	ILE
1	D	577	SER
1	D	585	GLU
1	D	596	ASN
1	D	610	LEU
1	D	624	LEU
1	D	685	ASN
1	D	689	LEU
1	D	692	ASP
1	D	714	THR
1	D	730	LYS
1	D	739	LEU
1	D	755	GLU
1	E	77	ARG
1	E	101	VAL
1	E	177	GLU
1	E	206	LYS
1	E	209	THR
1	E	220	GLN
1	E	237	PHE
1	E	284	GLN
1	E	319	LEU
1	E	363	SER
1	E	385	TRP
1	E	428	GLU
1	E	456	LYS
1	E	479	LYS
1	E	481	LEU
1	E	486	LYS
1	E	517	THR
1	E	519	GLN
1	E	553	LEU
1	E	564	MET
1	E	570	VAL
1	E	573	ILE
1	E	577	SER
1	E	585	GLU
1	E	596	ASN
1	E	610	LEU
1	E	624	LEU
1	E	643	GLU
1	E	685	ASN

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Mol	Chain	Res	Type
1	E	689	LEU
1	E	714	THR
1	E	730	LYS
1	E	739	LEU
1	E	755	GLU
1	F	21	ASP
1	F	77	ARG
1	F	101	VAL
1	F	177	GLU
1	F	206	LYS
1	F	220	GLN
1	F	237	PHE
1	F	284	GLN
1	F	319	LEU
1	F	349	THR
1	F	363	SER
1	F	385	TRP
1	F	456	LYS
1	F	479	LYS
1	F	481	LEU
1	F	504	LYS
1	F	505	GLU
1	F	517	THR
1	F	519	GLN
1	F	553	LEU
1	F	558	GLU
1	F	564	MET
1	F	570	VAL
1	F	573	ILE
1	F	577	SER
1	F	585	GLU
1	F	596	ASN
1	F	610	LEU
1	F	624	LEU
1	F	685	ASN
1	F	689	LEU
1	F	692	ASP
1	F	714	THR
1	F	715	LYS
1	F	730	LYS
1	F	739	LEU
1	F	753	SER

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Mol	Chain	Res	Type
1	F	755	GLU
1	G	77	ARG
1	G	101	VAL
1	G	177	GLU
1	G	206	LYS
1	G	209	THR
1	G	220	GLN
1	G	237	PHE
1	G	284	GLN
1	G	319	LEU
1	G	363	SER
1	G	385	TRP
1	G	443	GLU
1	G	479	LYS
1	G	481	LEU
1	G	505	GLU
1	G	517	THR
1	G	519	GLN
1	G	553	LEU
1	G	564	MET
1	G	570	VAL
1	G	573	ILE
1	G	585	GLU
1	G	596	ASN
1	G	604	ILE
1	G	610	LEU
1	G	624	LEU
1	G	685	ASN
1	G	689	LEU
1	G	714	THR
1	G	730	LYS
1	G	739	LEU
1	H	21	ASP
1	H	77	ARG
1	H	101	VAL
1	H	177	GLU
1	H	206	LYS
1	H	220	GLN
1	H	237	PHE
1	H	284	GLN
1	H	319	LEU
1	H	363	SER

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Mol	Chain	Res	Type
1	H	385	TRP
1	H	433	GLU
1	H	443	GLU
1	H	475	TYR
1	H	476	ARG
1	H	479	LYS
1	H	506	SER
1	H	517	THR
1	H	519	GLN
1	H	553	LEU
1	H	570	VAL
1	H	573	ILE
1	H	577	SER
1	H	585	GLU
1	H	596	ASN
1	H	604	ILE
1	H	610	LEU
1	H	624	LEU
1	H	685	ASN
1	H	689	LEU
1	H	714	THR
1	H	719	ARG
1	H	730	LYS
1	H	736	ARG
1	H	739	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (213) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	81	GLN
1	A	84	GLN
1	A	188	ASN
1	A	198	ASN
1	A	216	ASN
1	A	226	GLN
1	A	264	ASN
1	A	283	ASN
1	A	284	GLN
1	A	298	GLN
1	A	358	ASN
1	A	374	ASN

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Mol	Chain	Res	Type
1	A	397	ASN
1	A	398	ASN
1	A	431	HIS
1	A	446	ASN
1	A	519	GLN
1	A	593	ASN
1	A	599	HIS
1	A	685	ASN
1	A	695	ASN
1	A	700	ASN
1	A	709	ASN
1	A	716	ASN
1	B	59	GLN
1	B	81	GLN
1	B	188	ASN
1	B	198	ASN
1	B	216	ASN
1	B	226	GLN
1	B	246	ASN
1	B	264	ASN
1	B	283	ASN
1	B	358	ASN
1	B	374	ASN
1	B	397	ASN
1	B	398	ASN
1	B	431	HIS
1	B	446	ASN
1	B	519	GLN
1	B	581	GLN
1	B	596	ASN
1	B	599	HIS
1	B	685	ASN
1	B	695	ASN
1	B	700	ASN
1	B	709	ASN
1	B	716	ASN
1	C	59	GLN
1	C	103	GLN
1	C	188	ASN
1	C	216	ASN
1	C	226	GLN
1	C	264	ASN

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Mol	Chain	Res	Type
1	C	283	ASN
1	C	284	GLN
1	C	358	ASN
1	C	374	ASN
1	C	397	ASN
1	C	431	HIS
1	C	446	ASN
1	C	460	ASN
1	C	500	ASN
1	C	519	GLN
1	C	593	ASN
1	C	596	ASN
1	C	599	HIS
1	C	626	GLN
1	C	685	ASN
1	C	695	ASN
1	C	700	ASN
1	C	709	ASN
1	C	716	ASN
1	D	59	GLN
1	D	81	GLN
1	D	158	HIS
1	D	188	ASN
1	D	198	ASN
1	D	216	ASN
1	D	226	GLN
1	D	258	GLN
1	D	264	ASN
1	D	283	ASN
1	D	358	ASN
1	D	374	ASN
1	D	397	ASN
1	D	398	ASN
1	D	431	HIS
1	D	446	ASN
1	D	497	ASN
1	D	500	ASN
1	D	519	GLN
1	D	593	ASN
1	D	596	ASN
1	D	599	HIS
1	D	685	ASN

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Mol	Chain	Res	Type
1	D	695	ASN
1	D	700	ASN
1	D	709	ASN
1	D	713	HIS
1	D	716	ASN
1	E	59	GLN
1	E	81	GLN
1	E	103	GLN
1	E	188	ASN
1	E	198	ASN
1	E	226	GLN
1	E	258	GLN
1	E	264	ASN
1	E	283	ASN
1	E	358	ASN
1	E	369	GLN
1	E	397	ASN
1	E	398	ASN
1	E	431	HIS
1	E	446	ASN
1	E	460	ASN
1	E	497	ASN
1	E	500	ASN
1	E	519	GLN
1	E	593	ASN
1	E	596	ASN
1	E	599	HIS
1	E	685	ASN
1	E	695	ASN
1	E	700	ASN
1	E	709	ASN
1	E	713	HIS
1	E	716	ASN
1	F	59	GLN
1	F	81	GLN
1	F	188	ASN
1	F	198	ASN
1	F	216	ASN
1	F	226	GLN
1	F	264	ASN
1	F	283	ASN
1	F	284	GLN

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Mol	Chain	Res	Type
1	F	358	ASN
1	F	374	ASN
1	F	397	ASN
1	F	431	HIS
1	F	446	ASN
1	F	460	ASN
1	F	497	ASN
1	F	500	ASN
1	F	519	GLN
1	F	593	ASN
1	F	596	ASN
1	F	599	HIS
1	F	685	ASN
1	F	695	ASN
1	F	700	ASN
1	F	709	ASN
1	F	716	ASN
1	G	59	GLN
1	G	81	GLN
1	G	84	GLN
1	G	103	GLN
1	G	188	ASN
1	G	198	ASN
1	G	216	ASN
1	G	226	GLN
1	G	258	GLN
1	G	262	ASN
1	G	264	ASN
1	G	283	ASN
1	G	284	GLN
1	G	358	ASN
1	G	374	ASN
1	G	397	ASN
1	G	431	HIS
1	G	446	ASN
1	G	497	ASN
1	G	500	ASN
1	G	519	GLN
1	G	593	ASN
1	G	596	ASN
1	G	599	HIS
1	G	685	ASN

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Mol	Chain	Res	Type
1	G	695	ASN
1	G	700	ASN
1	G	709	ASN
1	G	716	ASN
1	H	59	GLN
1	H	81	GLN
1	H	84	GLN
1	H	103	GLN
1	H	188	ASN
1	H	198	ASN
1	H	216	ASN
1	H	226	GLN
1	H	258	GLN
1	H	264	ASN
1	H	283	ASN
1	H	284	GLN
1	H	358	ASN
1	H	374	ASN
1	H	397	ASN
1	H	431	HIS
1	H	446	ASN
1	H	460	ASN
1	H	500	ASN
1	H	519	GLN
1	H	593	ASN
1	H	596	ASN
1	H	599	HIS
1	H	685	ASN
1	H	695	ASN
1	H	700	ASN
1	H	709	ASN
1	H	716	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 8 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	D	802	-	5,5,5	0.41	0	5,5,5	0.24	0
3	SWA	G	801	2	13,13,13	1.18	1 (7%)	14,19,19	1.88	2 (14%)
4	GOL	F	802	-	5,5,5	0.38	0	5,5,5	0.50	0
4	GOL	E	803	-	5,5,5	0.41	0	5,5,5	0.45	0
4	GOL	A	803	-	5,5,5	0.47	0	5,5,5	1.32	0
3	SWA	F	801	2	13,13,13	0.73	0	14,19,19	0.89	0
4	GOL	A	805	-	5,5,5	0.35	0	5,5,5	0.67	0
3	SWA	D	801	2	13,13,13	1.21	1 (7%)	14,19,19	2.32	3 (21%)
3	SWA	C	801	2	13,13,13	0.91	0	14,19,19	2.08	4 (28%)
4	GOL	C	804	-	5,5,5	0.43	0	5,5,5	1.21	1 (20%)
4	GOL	A	806	-	5,5,5	0.43	0	5,5,5	0.32	0
4	GOL	B	804	-	5,5,5	0.49	0	5,5,5	1.12	0
4	GOL	B	802	-	5,5,5	0.38	0	5,5,5	0.70	0
3	SWA	E	801	2	13,13,13	0.78	0	14,19,19	1.98	3 (21%)
3	SWA	A	801	2	13,13,13	0.62	0	14,19,19	2.54	1 (7%)
4	GOL	D	804	-	5,5,5	0.42	0	5,5,5	0.55	0
4	GOL	C	802	-	5,5,5	0.43	0	5,5,5	0.25	0
4	GOL	A	802	-	5,5,5	0.35	0	5,5,5	0.20	0
3	SWA	H	801	2	13,13,13	1.07	1 (7%)	14,19,19	2.41	3 (21%)
3	SWA	B	801	2	13,13,13	0.93	1 (7%)	14,19,19	1.86	3 (21%)
4	GOL	A	804	-	5,5,5	0.60	0	5,5,5	1.34	1 (20%)
4	GOL	E	802	-	5,5,5	0.37	0	5,5,5	0.88	0
4	GOL	B	803	-	5,5,5	0.44	0	5,5,5	0.60	0
4	GOL	D	803	-	5,5,5	0.41	0	5,5,5	0.95	0
4	GOL	C	803	-	5,5,5	0.49	0	5,5,5	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	802	-	-	0/4/4/4	-
4	GOL	C	803	-	-	4/4/4/4	-
4	GOL	F	802	-	-	2/4/4/4	-
3	SWA	G	801	2	-	-	1/2/2/2
4	GOL	E	803	-	-	3/4/4/4	-
4	GOL	A	803	-	-	1/4/4/4	-
4	GOL	A	805	-	-	4/4/4/4	-
3	SWA	F	801	2	-	-	0/2/2/2
3	SWA	C	801	2	-	-	0/2/2/2
3	SWA	D	801	2	-	-	0/2/2/2
4	GOL	C	804	-	-	1/4/4/4	-
4	GOL	A	806	-	-	1/4/4/4	-
4	GOL	B	804	-	-	2/4/4/4	-
4	GOL	B	802	-	-	0/4/4/4	-
4	GOL	D	804	-	-	0/4/4/4	-
3	SWA	A	801	2	-	-	0/2/2/2
3	SWA	E	801	2	-	-	0/2/2/2
4	GOL	C	802	-	-	4/4/4/4	-
4	GOL	A	802	-	-	4/4/4/4	-
3	SWA	H	801	2	-	-	0/2/2/2
4	GOL	A	804	-	-	2/4/4/4	-
3	SWA	B	801	2	-	-	0/2/2/2
4	GOL	E	802	-	-	2/4/4/4	-
4	GOL	B	803	-	-	1/4/4/4	-
4	GOL	D	803	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	SWA	C2-C1	3.65	1.57	1.52
3	G	801	SWA	C7-C3	3.01	1.58	1.53
3	B	801	SWA	C8-C7	-2.30	1.49	1.53
3	H	801	SWA	C7-C3	2.23	1.57	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	SWA	C5-N4-C3	8.97	120.87	112.14
3	H	801	SWA	C5-N4-C3	6.77	118.73	112.14
3	D	801	SWA	C5-N4-C3	6.69	118.66	112.14
3	E	801	SWA	C5-N4-C3	5.79	117.77	112.14
3	B	801	SWA	C5-N4-C3	5.15	117.16	112.14
3	C	801	SWA	C5-N4-C3	4.84	116.85	112.14
3	H	801	SWA	C5-N4-C9	-4.58	104.48	115.29
3	G	801	SWA	C5-N4-C3	-4.50	107.75	112.14
3	G	801	SWA	C5-N4-C9	-3.88	106.14	115.29
3	D	801	SWA	C2-C1-C3	3.67	117.90	110.57
3	C	801	SWA	C2-C1-C3	3.13	116.83	110.57
3	E	801	SWA	O11-C7-C8	-2.86	105.19	111.97
3	D	801	SWA	C9-N4-C3	2.74	110.61	104.79
3	C	801	SWA	O11-C7-C8	-2.70	105.58	111.97
3	H	801	SWA	C9-N4-C3	-2.69	99.07	104.79
3	C	801	SWA	O13-C8-C7	-2.32	106.86	111.43
4	C	804	GOL	O2-C2-C3	2.23	118.41	109.18
3	B	801	SWA	O13-C8-C9	-2.20	105.77	110.94
4	A	804	GOL	O1-C1-C2	2.09	119.80	110.38
3	B	801	SWA	O11-C7-C8	-2.08	107.04	111.97
3	E	801	SWA	C2-C1-C3	2.07	114.70	110.57

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	802	GOL	O1-C1-C2-C3
4	A	802	GOL	C1-C2-C3-O3
4	A	805	GOL	O1-C1-C2-C3
4	A	805	GOL	C1-C2-C3-O3
4	B	804	GOL	O1-C1-C2-C3
4	C	802	GOL	O1-C1-C2-C3
4	C	802	GOL	C1-C2-C3-O3
4	D	803	GOL	C1-C2-C3-O3
4	E	802	GOL	O1-C1-C2-C3
4	E	803	GOL	C1-C2-C3-O3
4	F	802	GOL	C1-C2-C3-O3
4	A	804	GOL	C1-C2-C3-O3
4	C	803	GOL	O1-C1-C2-C3
4	C	803	GOL	C1-C2-C3-O3
4	D	803	GOL	O1-C1-C2-C3
4	A	802	GOL	O1-C1-C2-O2
4	A	802	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	805	GOL	O1-C1-C2-O2
4	A	805	GOL	O2-C2-C3-O3
4	B	804	GOL	O1-C1-C2-O2
4	C	802	GOL	O1-C1-C2-O2
4	C	803	GOL	O1-C1-C2-O2
4	E	802	GOL	O1-C1-C2-O2
4	E	803	GOL	O2-C2-C3-O3
4	C	802	GOL	O2-C2-C3-O3
4	D	803	GOL	O2-C2-C3-O3
4	F	802	GOL	O2-C2-C3-O3
4	A	806	GOL	C1-C2-C3-O3
4	B	803	GOL	O2-C2-C3-O3
4	C	803	GOL	O2-C2-C3-O3
4	D	803	GOL	O1-C1-C2-O2
4	A	803	GOL	O1-C1-C2-O2
4	C	804	GOL	O1-C1-C2-C3
4	E	803	GOL	O1-C1-C2-O2
4	A	804	GOL	O2-C2-C3-O3

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	801	SWA	C1-C2-C3-C5-C6-N4

15 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	802	GOL	2	0
3	G	801	SWA	5	0
4	A	803	GOL	2	0
3	F	801	SWA	5	0
3	D	801	SWA	5	0
3	C	801	SWA	4	0
4	B	804	GOL	4	0
3	E	801	SWA	1	0
3	A	801	SWA	2	0
4	D	804	GOL	2	0
3	H	801	SWA	5	0
3	B	801	SWA	2	0
4	A	804	GOL	1	0
4	B	803	GOL	2	0
4	C	803	GOL	6	0

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	736/744 (98%)	-0.66	0 100 100	7, 12, 20, 24	3 (0%)
1	B	736/744 (98%)	-0.55	0 100 100	7, 12, 20, 25	5 (0%)
1	C	737/744 (99%)	-0.55	1 (0%) 92 90	7, 12, 20, 29	2 (0%)
1	D	738/744 (99%)	-0.51	2 (0%) 90 86	7, 12, 20, 36	2 (0%)
1	E	736/744 (98%)	-0.17	1 (0%) 92 90	7, 12, 19, 26	2 (0%)
1	F	736/744 (98%)	-0.12	4 (0%) 87 82	7, 12, 19, 24	1 (0%)
1	G	736/744 (98%)	-0.01	4 (0%) 87 82	7, 12, 19, 24	0
1	H	736/744 (98%)	0.26	7 (0%) 79 72	7, 12, 19, 24	0
All	All	5891/5952 (98%)	-0.29	19 (0%) 90 86	7, 12, 19, 36	15 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	216[A]	ASN	3.4
1	H	580	GLY	2.8
1	C	756	LEU	2.6
1	H	717	TYR	2.6
1	H	207	PRO	2.5
1	F	452	PRO	2.4
1	H	533	GLU	2.4
1	F	580	GLY	2.4
1	G	441	GLY	2.3
1	F	491	PHE	2.3
1	H	102	GLY	2.3
1	G	668	GLU	2.2
1	G	749	PRO	2.2
1	D	216	ASN	2.2
1	H	723	LEU	2.1
1	D	757	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	755	GLU	2.1
1	G	613	TYR	2.0
1	F	105	VAL	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	C	802	6/6	0.71	0.21	59,60,60,61	0
3	SWA	H	801	12/12	0.76	0.18	25,27,30,33	0
4	GOL	D	804	6/6	0.80	0.14	29,30,31,34	0
4	GOL	C	803	6/6	0.81	0.14	32,33,34,34	0
3	SWA	G	801	12/12	0.81	0.16	39,40,42,45	0
4	GOL	E	803	6/6	0.85	0.14	38,39,39,39	0
4	GOL	C	804	6/6	0.86	0.15	32,33,33,35	0
4	GOL	B	804	6/6	0.89	0.11	22,26,26,28	0
4	GOL	A	806	6/6	0.89	0.11	42,43,44,45	0
4	GOL	A	804	6/6	0.90	0.13	19,19,21,22	0
4	GOL	B	802	6/6	0.90	0.13	29,30,30,31	0
4	GOL	B	803	6/6	0.90	0.13	45,45,46,47	0
4	GOL	F	802	6/6	0.90	0.12	30,32,33,33	0
4	GOL	A	803	6/6	0.91	0.13	32,35,35,36	0
4	GOL	E	802	6/6	0.91	0.10	30,31,31,31	0
4	GOL	D	802	6/6	0.91	0.16	30,33,34,36	0
4	GOL	D	803	6/6	0.91	0.10	32,33,35,35	0
3	SWA	A	801	12/12	0.92	0.12	37,39,40,41	0
2	CA	H	800	1/1	0.92	0.17	43,43,43,43	0
3	SWA	F	801	12/12	0.93	0.12	22,24,24,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	E	800	1/1	0.93	0.07	33,33,33,33	0
4	GOL	A	805	6/6	0.93	0.08	31,33,34,34	0
3	SWA	D	801	12/12	0.93	0.11	17,18,20,21	0
4	GOL	A	802	6/6	0.94	0.08	42,43,44,45	0
3	SWA	C	801	12/12	0.95	0.12	18,21,22,24	0
2	CA	A	800	1/1	0.95	0.08	28,28,28,28	0
3	SWA	B	801	12/12	0.96	0.09	9,14,15,17	0
3	SWA	E	801	12/12	0.97	0.10	8,11,13,14	0
2	CA	C	800	1/1	0.97	0.07	23,23,23,23	0
2	CA	D	800	1/1	0.97	0.07	30,30,30,30	0
2	CA	G	800	1/1	0.98	0.16	39,39,39,39	0
2	CA	B	800	1/1	0.98	0.06	11,11,11,11	0
2	CA	F	800	1/1	0.98	0.12	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.