Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 12:37 am GMT

PDB ID	:	2WW0
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:

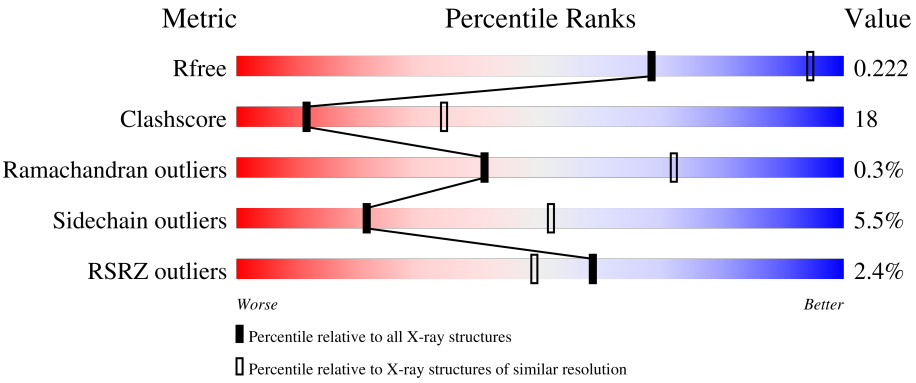
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	71% 25%
1	B	744	71% 25%
1	C	744	72% 23%
1	D	744	70% 26%
1	E	744	% 72% 24%

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Mol	Chain	Length	Quality of chain
1	F	744	2% 69% 27%
1	G	744	5% 68% 28%
1	H	744	10% 66% 30%

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 (three-letter code: 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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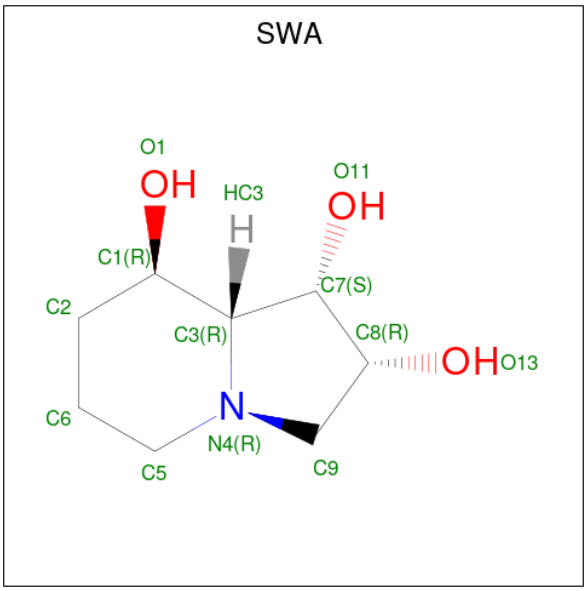
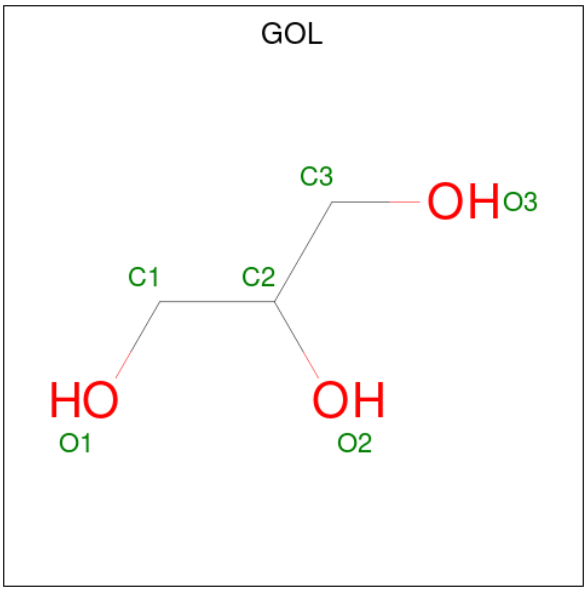
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0

- Molecule 3 is 1S-8AB-OCTAHYDRO-INDOLIZIDINE-1A,2A,8B-TRIOL (three-letter code: SWA) (formula: $C_8H_{15}NO_3$).



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

- Molecule 4 is GLYCEROL (three-letter code: 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 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

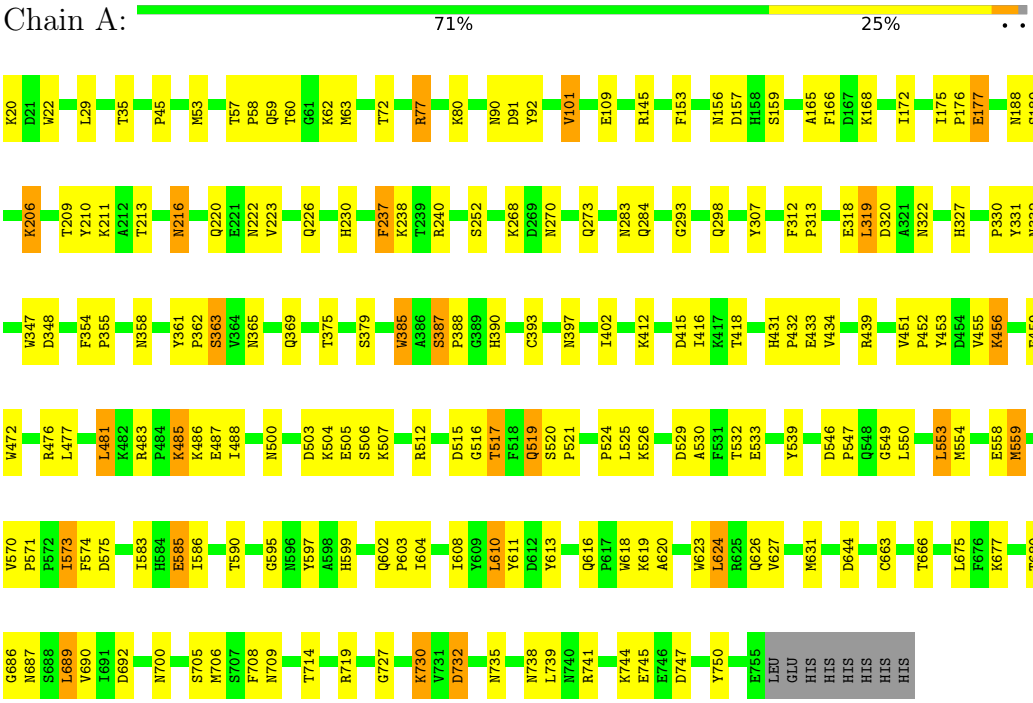
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	117	Total O 117 117	0	0
5	B	105	Total O 105 105	0	0
5	C	80	Total O 80 80	0	0
5	D	110	Total O 110 110	0	0
5	E	77	Total O 77 77	0	0
5	F	42	Total O 42 42	0	0
5	G	6	Total O 6 6	0	0
5	H	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

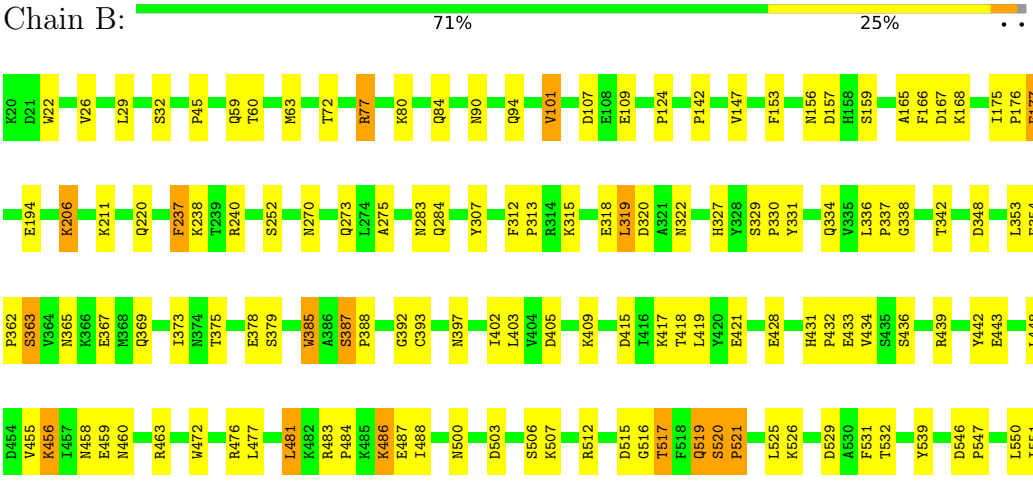
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

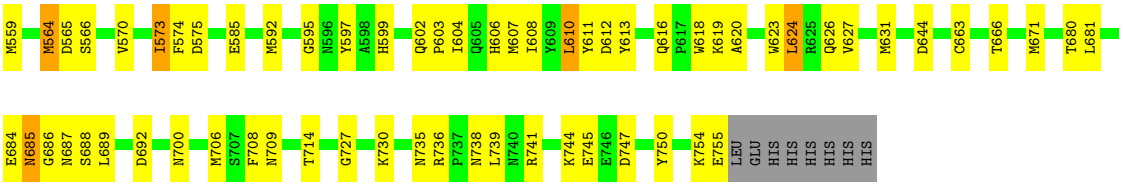
Chain A:



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

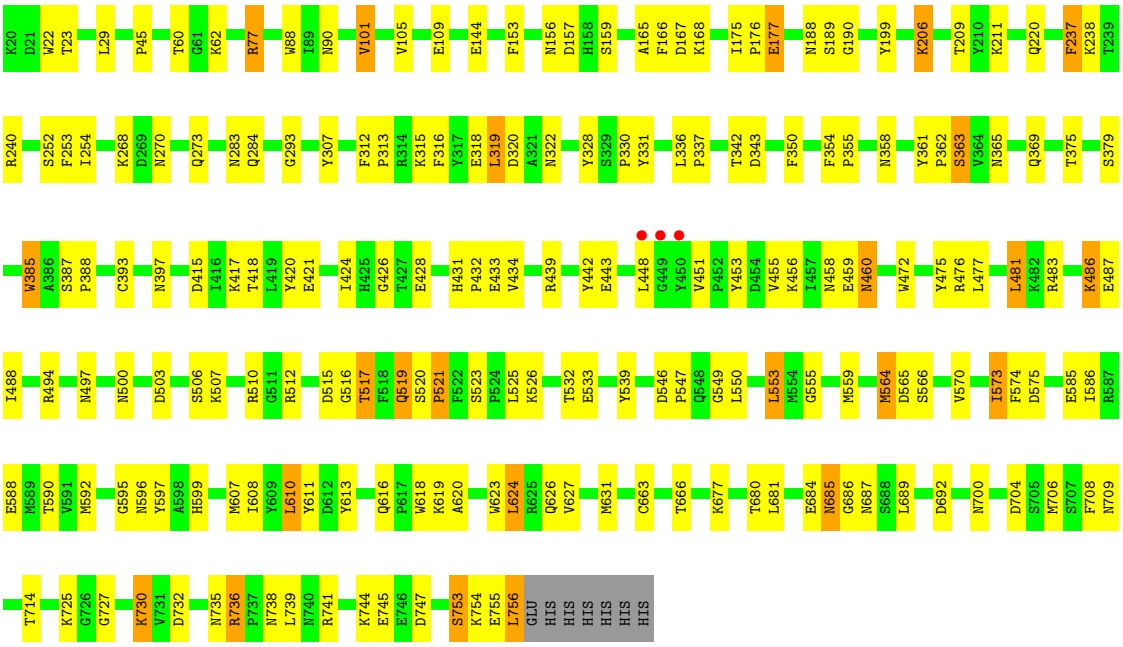
Chain B:





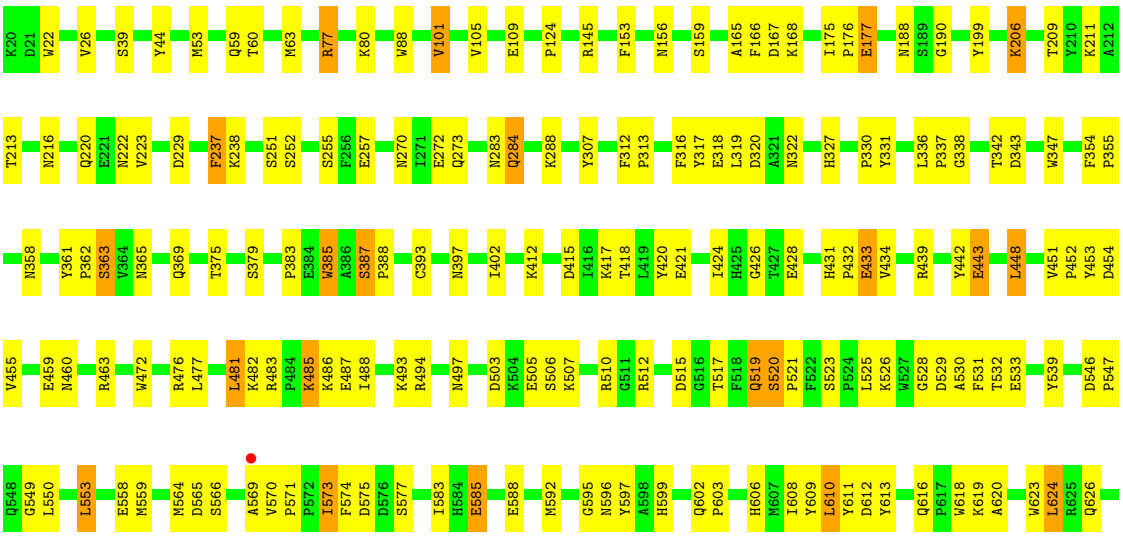
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

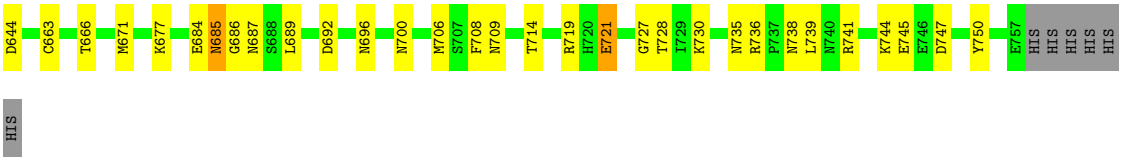
Chain C:



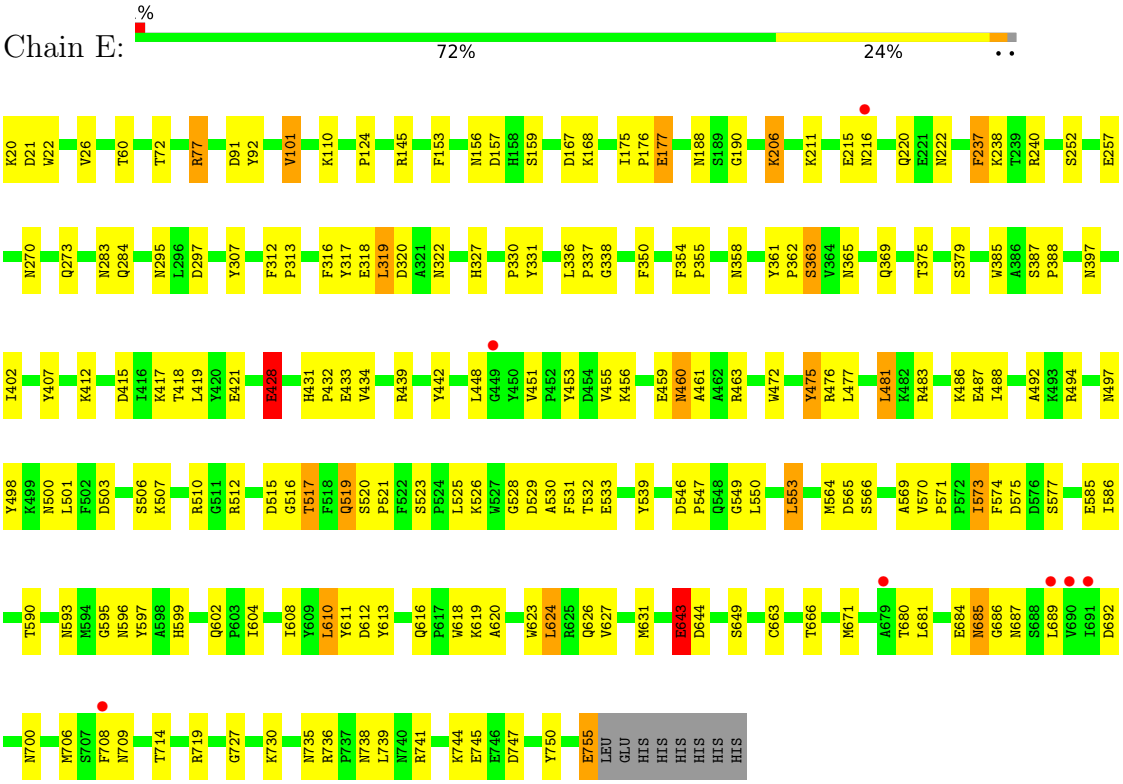
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain D:

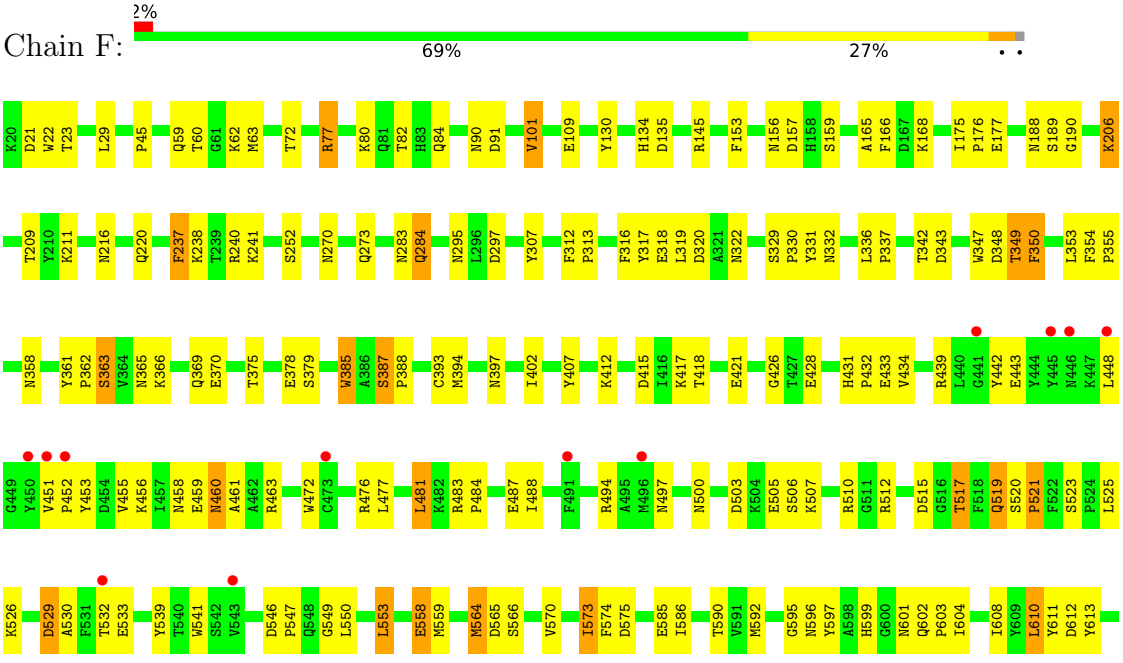


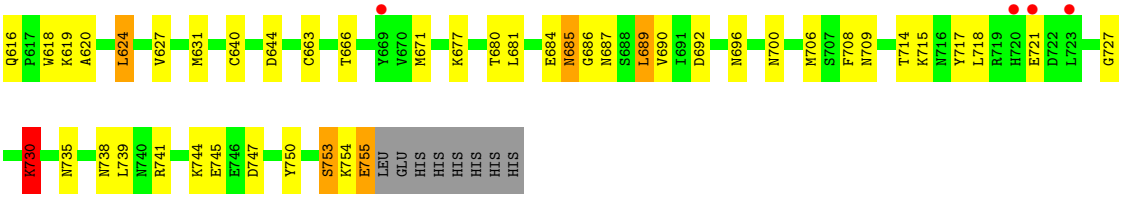


• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE



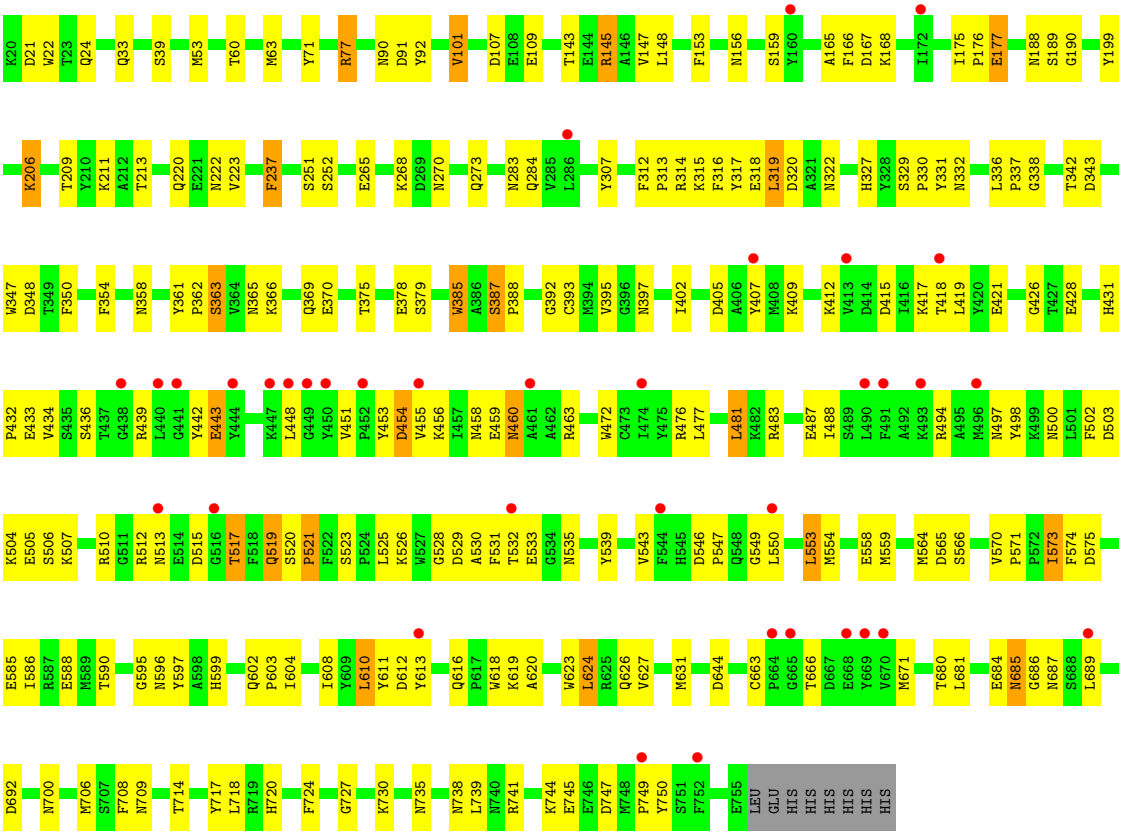
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE





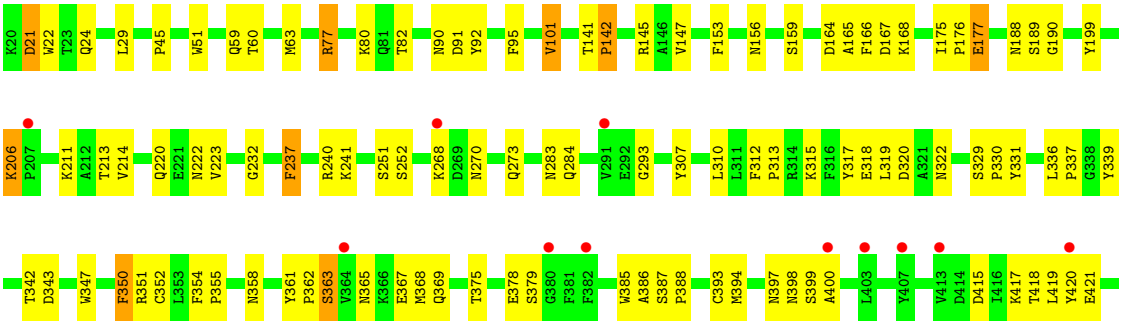
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

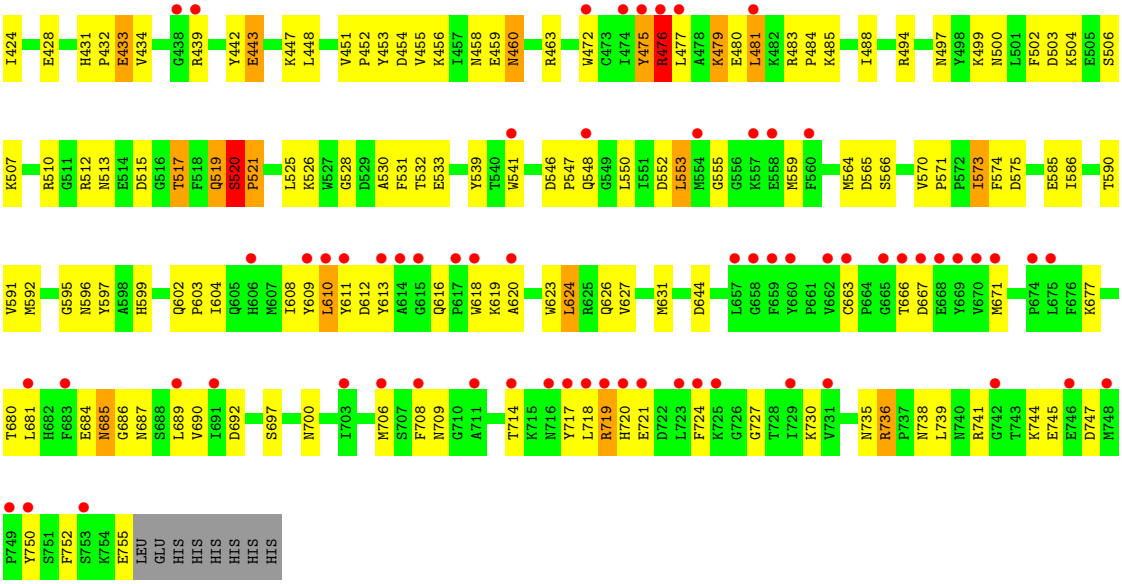
Chain G:



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

Chain H:




I424 E428 H431 P432 E433 V434 G438 R439 Y442 E443 K447 L448 V451 P452 Y453 D454 V455 K456 I457 N458 E459 N460 R463 W472 C473 I474 Y475 R476 L477 A478 K479 E480 L481 K482 R483 P484 K485 I488 R494 N497 Y498 K499 N500 L501 F502 D503 K504 E505 S506
K507 R510 G511 R512 N513 E514 D515 G516 T517 F518 Q519 S520 P521 L525 K526 W527 G528 D529 A530 F531 T532 E533 Y539 T540 W541 D546 P547 Q548 G549 L550 I551 D552 L553 M554 G555 G556 K557 E558 M559 F560 M564 D565 S566 V570 P571 P572 I573 F574 D575 E585 I586 T590
V591 M592 G595 N596 Y597 A598 H599 Q602 P603 I604 Q605 H606 M607 I608 Y609 L610 Y611 D612 Y613 A614 G615 Q616 P617 W618 K619 A620 W623 L624 R625 Q626 V627 M631 D644 L657 G658 F659 Y660 P661 V662 C663 P664 G665 T666 D667 E668 Y669 V670 M671 P674 L675 F676 K677
T680 L681 H682 F683 E684 N685 G686 N687 S688 L689 V690 I691 D692 S697 N700 I703 M706 S707 F708 N709 G710 A711 T714 K715 N716 Y717 L718 R719 H720 E721 D722 L723 F724 K725 G726 G727 T728 I729 K730 V731 N735 R736 P737 N738 L739 N740 R741 G742 T743 K744 E745 E746 D747 M748
P749 Y750 S751 F752 S753 K754 E755 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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 65.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (218.23-2.80) 97.9 (65.61-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.81Å)	Xtriage
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 (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	48426	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.58	0/6167	0.64	2/8365 (0.0%)
1	B	0.60	0/6193	0.63	2/8398 (0.0%)
1	C	0.57	0/6166	0.63	2/8365 (0.0%)
1	D	0.60	1/6171 (0.0%)	0.65	4/8373 (0.0%)
1	E	0.57	1/6143 (0.0%)	0.64	1/8337 (0.0%)
1	F	0.51	0/6138	0.61	3/8330 (0.0%)
1	G	0.46	0/6113	0.60	5/8303 (0.1%)
1	H	0.49	1/6079 (0.0%)	0.62	4/8265 (0.0%)
All	All	0.55	3/49170 (0.0%)	0.63	23/66736 (0.0%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	721	GLU	CG-CD	5.88	1.60	1.51
1	E	428	GLU	CG-CD	5.38	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	476	ARG	NE-CZ	5.28	1.40	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	448	LEU	CA-CB-CG	-7.07	99.05	115.30
1	G	145	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	B	211	LYS	CD-CE-NZ	6.31	126.20	111.70
1	E	643	GLU	CA-CB-CG	6.28	127.22	113.40
1	C	730	LYS	CB-CG-CD	6.27	127.91	111.60
1	C	211	LYS	CD-CE-NZ	6.25	126.07	111.70
1	F	387	SER	C-N-CD	-6.22	106.91	120.60
1	F	211	LYS	CD-CE-NZ	6.17	125.90	111.70
1	H	520	SER	C-N-CD	-5.91	107.60	120.60
1	A	387	SER	C-N-CD	-5.59	108.30	120.60
1	G	387	SER	C-N-CD	-5.52	108.46	120.60
1	G	145	ARG	NH1-CZ-NH2	5.50	125.45	119.40
1	D	387	SER	C-N-CD	-5.47	108.56	120.60
1	A	730	LYS	CB-CG-CD	5.44	125.74	111.60
1	D	730	LYS	CB-CG-CD	5.44	125.73	111.60
1	H	481	LEU	CB-CG-CD1	5.42	120.22	111.00
1	B	387	SER	C-N-CD	-5.30	108.94	120.60
1	D	454	ASP	CB-CG-OD1	5.23	123.01	118.30
1	F	730	LYS	CB-CG-CD	5.22	125.16	111.60
1	H	521	PRO	N-CA-C	-5.21	98.56	112.10
1	G	454	ASP	CB-CG-OD1	5.12	122.91	118.30
1	G	145	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	H	476	ARG	NE-CZ-NH1	5.06	122.83	120.30

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

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Mol	Chain	Res	Type	Group
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	180	0
1	B	5997	0	5677	199	0
1	C	5979	0	5652	165	0
1	D	5984	0	5647	194	0
1	E	5956	0	5614	173	0
1	F	5954	0	5610	220	0
1	G	5932	0	5554	236	0
1	H	5899	0	5483	274	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	3	0
3	B	12	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	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	1638	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 18.

All (1638) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592[B]:MET:CE	1:B:631:MET:HE1	1.22	1.60
1:C:592[B]:MET:CE	1:C:631:MET:HE1	1.27	1.59
1:B:592[B]:MET:HE2	1:B:631:MET:CE	1.20	1.58
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:H:472:TRP:CZ2	1:H:476:ARG:HD3	1.46	1.51
1:H:472:TRP:CZ2	1:H:476:ARG:CD	1.94	1.49
1:C:592[B]:MET:HE2	1:C:631:MET:CE	1.40	1.49
1:G:507:LYS:NZ	1:G:559:MET:HE1	1.13	1.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:573:ILE:CD1	1:D:574:PHE:H	1.34	1.39
1:H:483:ARG:O	1:H:488:ILE:CD1	1.71	1.37
1:A:507:LYS:NZ	1:A:559:MET:HE2	1.34	1.36
1:F:730:LYS:HE2	5:F:2042:HOH:O	1.23	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:B:592[B]:MET:CE	1:B:631:MET:CE	1.92	1.25
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: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: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: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
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:G:363:SER:OG	1:G:684:GLU:CD	1.83	1.17
1:F:677:LYS:NZ	1:F:696:ASN:O	1.79	1.16
1:H:476:ARG:HB3	1:H:476:ARG:NH1	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:E:415:ASP:OD2	1:E:418:THR:OG1	1.67	1.12
1:G:507:LYS:HZ2	1:G:559:MET:CE	1.59	1.11
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:G:706:MET:HE3	1:G:741:ARG:HH22	1.17	1.09
1:H:483:ARG:C	1:H:488:ILE:HD11	1.73	1.09
1:E:706:MET:HE3	1:E:741:ARG:HH22	1.16	1.08
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:546:ASP:CG	1:F:753:SER:OG	1.94	1.05
1:H:484:PRO:C	1:H:488:ILE:HD12	1.76	1.05
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: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
1:C:592[B]:MET:CE	1:C:631:MET:CE	2.08	1.02
1:H:472:TRP:HH2	1:H:476:ARG:HE	1.05	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:C:706:MET:HE3	1:C:741:ARG:HH22	1.25	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: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:F:706:MET:HE3	1:F:741:ARG:HH22	1.25	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:507:LYS:HZ1	1:A:559:MET:CE	1.77	0.97
1:F:503:ASP:OD2	1:F:506:SER:OG	1.79	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:D:363:SER:OG	1:D:684:GLU:CD	2.03	0.96
1:F:550:LEU:HA	1:F:553:LEU:CD1	1.95	0.96
1:G:507:LYS:CE	1:G:559:MET:HE1	1.89	0.96
1:H:472:TRP:CH2	1:H:476:ARG:CD	2.32	0.96
1:G:442:TYR:CD2	1:G:443:GLU:OE2	2.18	0.95
3:G:801:SWA:HC52	3:G:801:SWA:O13	1.62	0.95
1:B:592[B]:MET:HE1	1:B:631:MET:CE	1.96	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:B:592[B]:MET:CE	1:B:631:MET:HE2	1.95	0.94
1:D:685:ASN:C	1:D:685:ASN:HD22	1.64	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:C:546:ASP:OD1	1:C:753:SER:OG	1.85	0.94
1:H:706:MET:HE3	1:H:741:ARG:HH22	1.33	0.94
1:D:684:GLU:OE2	4:D:804:GOL:O3	1.85	0.94
1:A:550:LEU:HA	1:A:553:LEU:HD12	1.50	0.93
1:F:592[B]:MET:CE	1:F:631:MET:HE1	1.99	0.93
1:C:157:ASP:OD1	1:C:238:LYS:HE3	1.69	0.92
1:D:685:ASN:HD22	1:D:686:GLY:N	1.66	0.92
1:E:706:MET:HE3	1:E:741:ARG:NH2	1.85	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:B:706:MET:HE3	1:B:741:ARG:HH22	1.32	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:G:507:LYS:HE3	1:G:559:MET:HE2	1.51	0.90
1:H:329:SER:OG	1:H:378:GLU:OE1	1.87	0.90
1:H:573:ILE:CD1	1:H:574:PHE:H	1.79	0.90
1:G:507:LYS:CE	1:G:559:MET:HE3	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:347:TRP:CZ3	3:H:801:SWA:HC7	2.07	0.90
1:G:507:LYS:HE3	1:G:559:MET:HE3	1.54	0.90
1:F:546:ASP:CG	1:F:753:SER:HG	1.71	0.90
1:H:608:ILE:HG21	1:H:624:LEU:HD13	1.54	0.90
1:A:252:SER:OG	1:A:318:GLU:OE1	1.90	0.89
1:H:685:ASN:C	1:H:685:ASN:HD22	1.75	0.89
1:F:730:LYS:CE	5:F:2042:HOH:O	1.94	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
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: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: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:H:555:GLY:O	1:H:559:MET:HE3	1.75	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:G:685:ASN:C	1:G:685:ASN:HD22	1.76	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:685:ASN:HD22	1:F:685:ASN:C	1.77	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:HD3	1:B:486:LYS:H	1.39	0.86
1:G:407:TYR:CE2	1:G:412:LYS:HD3	2.11	0.86
1:A:685:ASN:HD22	1:A:685:ASN:C	1.76	0.86
1:C:375:THR:O	1:C:379:SER:OG	1.94	0.86
1:A:706:MET:HE3	1:A:741:ARG:HH22	1.40	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:G:706:MET:HE3	1:G:741:ARG:NH2	1.91	0.85
1:H:685:ASN:ND2	1:H:687:ASN:H	1.72	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:507:LYS:NZ	1:D:559:MET:HE2	1.92	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:706:MET:HE3	1:C:741:ARG:NH2	1.93	0.84
1:D:507:LYS:NZ	1:D:559:MET:CE	2.40	0.84
1:B:547:PRO:HG2	1:B:613:TYR:CE2	2.13	0.84
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:E:363:SER:OG	1:E:684:GLU:CD	2.16	0.84
1:B:375:THR:O	1:B:379:SER:OG	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:A:397:ASN:ND2	1:A:439:ARG:HE	1.77	0.83
1:D:363:SER:OG	1:D:684:GLU:OE2	1.94	0.83
1:H:347:TRP:HZ3	3:H:801:SWA:HC7	1.44	0.83
1:D:573:ILE:HD12	1:D:574:PHE:H	0.66	0.83
1:E:685:ASN:C	1:E:685:ASN:HD22	1.81	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: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: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:363:SER:OG	1:B:684:GLU:CD	2.17	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:C:685:ASN:C	1:C:685:ASN:HD22	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:503:ASP:OD2	1:G:506:SER:OG	1.99	0.80
1:D:685:ASN:C	1:D:685:ASN:ND2	2.35	0.79
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:A:507:LYS:HZ3	1:A:559:MET:HE2	1.44	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:E:415:ASP:CG	1:E:418:THR:OG1	2.22	0.79
1:C:608:ILE:HG21	1:C:624:LEU:HD13	1.65	0.78
1:G:507:LYS:HZ1	1:G:559:MET:HE1	1.45	0.78
1:G:573:ILE:HD12	1:G:574:PHE:H	0.78	0.78
1:B:685:ASN:C	1:B:685:ASN:HD22	1.86	0.78
1:F:348:ASP:OD1	3:F:801:SWA:O1	2.00	0.78
1:F:592[B]:MET:CE	1:F:592[B]:MET:HA	2.12	0.78
1:A:397:ASN:HD22	1:A:439:ARG:NE	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:706:MET:CE	1:G:741:ARG:HH22	1.96	0.78
1:F:706:MET:HE3	1:F:741:ARG:NH2	1.99	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:H:592:MET:SD	1:H:631:MET:CE	2.73	0.77
1:B:397:ASN:HD22	1:B:439:ARG:HE	1.32	0.77
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:E:706:MET:CE	1:E:741:ARG:NH2	2.47	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:B:706:MET:HE3	1:B:741:ARG:NH2	1.99	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	0.76
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:D:507:LYS:HZ2	1:D:559:MET:HE2	1.48	0.76
1:E:706:MET:CE	1:E:741:ARG:HH22	1.97	0.76
1:G:706:MET:CE	1:G:741:ARG:NH2	2.48	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:F:706:MET:CE	1:F:741:ARG:HH22	1.99	0.76
1:C:573:ILE:HD12	1:C:574:PHE:H	0.76	0.76
1:C:592[B]:MET:HE1	1:C:631:MET:CE	2.14	0.75
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:B:315:LYS:HZ1	4:B:804:GOL:H32	1.49	0.75
1:H:476:ARG:HB3	1:H:476:ARG:HH11	1.50	0.75
1:H:592:MET:SD	1:H:631:MET:HE1	2.26	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:F:442:TYR:CE1	1:F:443:GLU:OE2	2.39	0.74
1:H:442:TYR:CD1	1:H:443:GLU:OE2	2.40	0.74
1:F:706:MET:CE	1:F:741:ARG:NH2	2.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:592:MET:HA	1:H:592:MET:CE	2.18	0.74
1:H:608:ILE:CG2	1:H:624:LEU:HD13	2.16	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:D:706:MET:HE3	1:D:741:ARG:HH22	1.51	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
1:F:431:HIS:HD2	1:F:433:GLU:H	1.33	0.74
1:H:442:TYR:CE2	1:H:443:GLU:OE2	2.41	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:B:22:TRP:H	1:B:283:ASN:ND2	1.84	0.73
1:F:715:LYS:HE2	1:F:717:TYR:CE1	2.22	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:A:211:LYS:NZ	1:A:222:ASN:OD1	2.21	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:566:SER:O	1:B:570:VAL:HG13	1.88	0.73
1:G:405:ASP:CG	1:G:409:LYS:HZ1	1.92	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:F:252:SER:OG	1:F:318:GLU:CD	2.27	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:H:431:HIS:HD2	1:H:433:GLU:H	1.35	0.72
1:H:592:MET:HA	1:H:592:MET:HE1	1.72	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:HIS:HD2	1:E:433:GLU:H	1.38	0.71
1:B:706:MET:CE	1:B:741:ARG:NH2	2.54	0.71
1:G:331:TYR:CZ	1:G:375:THR:HG23	2.26	0.71
1:C:706:MET:CE	1:C:741:ARG:NH2	2.53	0.71
1:H:503:ASP:CG	1:H:506:SER:OG	2.29	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:483:ARG:O	1:G:488:ILE:HD11	1.91	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: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: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:H:533:GLU:OE2	3:H:801:SWA:HC8	1.92	0.70
1:H:706:MET:HE3	1:H:741:ARG:NH2	2.06	0.70
1:B:363:SER:OG	1:B:684:GLU:OE1	2.08	0.70
1:G:680:THR:C	1:G:681:LEU:HD23	2.12	0.70
1:B:608:ILE:CG2	1:B:624:LEU:HD13	2.22	0.70
1:F:331:TYR:CE2	1:F:375:THR:HG23	2.27	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:F:503:ASP:CG	1:F:506:SER:OG	2.29	0.69
1:H:442:TYR:CG	1:H:443:GLU:OE2	2.45	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:G:564:MET:HE1	1:G:610:LEU:HB2	1.73	0.69
1:F:592[B]:MET:CE	1:F:592[B]:MET:CA	2.69	0.69
1:F:685:ASN:ND2	1:F:685:ASN:C	2.45	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: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:B:564:MET:HE1	1:B:610:LEU:HB2	1.74	0.69
1:F:363:SER:OG	1:F:684:GLU:OE2	2.11	0.69
1:H:685:ASN:C	1:H:685:ASN:ND2	2.45	0.69
1:F:503:ASP:CG	1:F:506:SER:HG	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:515:ASP:OD1	1:F:517:THR:OG1	2.10	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:F:592[B]:MET:HE2	1:F:631:MET:HE1	1.75	0.68
1:H:472:TRP:CE2	1:H:476:ARG:HD2	2.19	0.68
1:B:515:ASP:OD1	1:B:515:ASP:C	2.32	0.68
1:E:744:LYS:HB2	1:E:747:ASP:OD2	1.93	0.68
1:G:550:LEU:O	1:G:553:LEU:HD22	1.93	0.68
1:C:503:ASP:CG	1:C:506:SER:OG	2.30	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: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:F:592[B]:MET:HA	1:F:592[B]:MET:HE3	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: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: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:515:ASP:OD1	1:E:515:ASP:C	2.32	0.67
1:H:550:LEU:HD12	1:H:553:LEU:HD12	1.76	0.67
1:H:680:THR:C	1:H:681:LEU:HD23	2.15	0.67
1:F:755:GLU:OE1	1:F:755:GLU:C	2.33	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
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:C:431:HIS:CD2	1:C:433:GLU:H	2.13	0.66
1:D:167:ASP:O	1:D:168:LYS:HB2	1.94	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:F:188:ASN:HD22	1:F:190:GLY:H	1.43	0.66
1:H:472:TRP:CZ3	1:H:476:ARG:HD3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:415:ASP:CG	1:G:418:THR:OG1	2.34	0.66
1:H:350:PHE:C	1:H:350:PHE:CD2	2.69	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:G:685:ASN:ND2	1:G:685:ASN:C	2.44	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:F:21:ASP:C	1:F:21:ASP:OD1	2.34	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:G:681:LEU:HD23	1:G:681:LEU:N	2.10	0.66
1:A:507:LYS:CE	1:A:559:MET:HE2	2.26	0.65
1:A:515:ASP:C	1:A:515:ASP:OD1	2.33	0.65
1:C:363:SER:OG	1:C:684:GLU:CD	2.34	0.65
1:C:573:ILE:CD1	1:C:574:PHE:N	2.46	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:G:550:LEU:C	1:G:553:LEU:HD22	2.15	0.65
1:H:252:SER:HG	1:H:318:GLU:CD	1.96	0.65
1:B:506:SER:O	1:B:507:LYS:HB2	1.94	0.65
1:D:573:ILE:HD12	1:D:573:ILE:C	2.06	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:C:515:ASP:C	1:C:515:ASP:OD1	2.31	0.65
1:G:442:TYR:CE1	1:G:443:GLU:CD	2.69	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:G:331:TYR:CE2	1:G:375:THR:HG23	2.31	0.65
1:F:483:ARG:O	1:F:488:ILE:HD11	1.95	0.65
1:H:706:MET:CE	1:H:741:ARG:NH2	2.60	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:507:LYS:HE3	1:F:559:MET:HE2	1.78	0.64
1:C:397:ASN:HD22	1:C:439:ARG:NE	1.92	0.64
1:A:706:MET:HE3	1:A:741:ARG:NH2	2.10	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:H:448:LEU:N	1:H:448:LEU:HD22	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: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:D:443:GLU:N	1:D:443:GLU:OE2	2.27	0.64
1:H:525:LEU:HD13	1:H:573:ILE:HG23	1.78	0.64
1:A:564:MET:HE1	1:A:610:LEU:HB2	1.79	0.63
1:C:525:LEU:HD13	1:C:573:ILE:HG23	1.79	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:H:681:LEU:HD23	1:H:681:LEU:N	2.12	0.63
1:H:484:PRO:C	1:H:488:ILE:CD1	2.61	0.63
1:A:706:MET:CE	1:A:741:ARG:NH2	2.61	0.63
1:D:507:LYS:HZ1	1:D:559:MET:HE1	1.62	0.63
1:F:363:SER:OG	1:F:684:GLU:CD	2.37	0.63
1:G:565:ASP:OD2	1:G:619:LYS:NZ	2.31	0.63
1:A:597:TYR:OH	1:A:599:HIS:HD2	1.82	0.63
1:A:685:ASN:C	1:A:685:ASN:ND2	2.45	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:C:685:ASN:ND2	1:C:685:ASN:C	2.52	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:405:ASP:CG	1:G:409:LYS:NZ	2.51	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:A:507:LYS:HZ1	1:A:559:MET:HE2	0.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:GLU:OE1	1:A:745:GLU:C	2.37	0.63
1:C:459:GLU:HG2	1:C:532:THR:HG22	1.80	0.63
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:H:415:ASP:CG	1:H:418:THR:OG1	2.37	0.62
1:H:555:GLY:O	1:H:559:MET:HE2	1.98	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:B:507:LYS:HE3	1:B:559[B]:MET:HE2	1.82	0.62
1:C:566:SER:O	1:C:570:VAL:HG13	1.99	0.62
1:C:363:SER:OG	1:C:684:GLU:OE1	2.17	0.62
1:D:503:ASP:OD1	1:D:503:ASP:C	2.39	0.62
1:H:564:MET:HE1	1:H:610:LEU:HB2	1.80	0.62
1:C:755:GLU:O	1:C:756:LEU:C	2.37	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
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:A:706:MET:CE	1:A:741:ARG:HH22	2.13	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:G:147:VAL:HG22	1:G:148:LEU:N	2.15	0.61
1:H:472:TRP:CZ3	1:H:476:ARG:NE	2.60	0.61
1:E:745:GLU:C	1:E:745:GLU:OE1	2.39	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: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:H:428:GLU:O	1:H:442:TYR:CZ	2.53	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:515:ASP:OD1	1:D:515:ASP:C	2.37	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: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:F:415:ASP:CG	1:F:418:THR:OG1	2.39	0.60
1:B:397:ASN:ND2	1:B:439:ARG:HE	1.99	0.60
1:D:505:GLU:HG2	1:D:506:SER:N	2.16	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: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:H:476:ARG:CB	1:H:476:ARG:HH11	2.08	0.60
1:H:745:GLU:OE1	1:H:745:GLU:C	2.40	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:350:PHE:C	1:F:350:PHE:CD2	2.75	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:84:GLN:HG3	1:F:90:ASN:C	2.22	0.60
1:F:715:LYS:HE2	1:F:717:TYR:HH	1.63	0.60
1:G:483:ARG:HB3	1:G:487:GLU:OE2	2.02	0.60
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:HG23	1:G:604:ILE:O	2.02	0.59
1:E:564:MET:HE1	1:E:610:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LYS:HE2	5:B:2032:HOH:O	2.02	0.59
1:C:709:ASN:HD21	1:C:727:GLY:HA3	1.67	0.59
1:G:745:GLU:C	1:G:745:GLU:OE1	2.40	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:D:564:MET:HE1	1:D:610:LEU:HB2	1.85	0.59
1:H:591:VAL:HG23	1:H:592:MET:HE2	1.83	0.59
1:A:363:SER:OG	1:A:684:GLU:OE2	2.20	0.59
1:D:415:ASP:CG	1:D:418:THR:OG1	2.41	0.59
1:E:472:TRP:O	1:E:476:ARG:HG2	2.02	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:H:443:GLU:CD	1:H:443:GLU:H	2.07	0.58
1:B:109:GLU:HB2	1:E:110:LYS:HZ1	1.65	0.58
1:G:500:ASN:O	1:G:512:ARG:NH1	2.35	0.58
1:H:320:ASP:OD1	1:H:320:ASP:C	2.42	0.58
1:A:358:ASN:HD21	1:A:365:ASN:HD22	1.51	0.58
1:A:431:HIS:HE1	5:A:2117:HOH:O	1.85	0.58
1:B:685:ASN:ND2	1:B:685:ASN:C	2.55	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:745:GLU:C	1:B:745:GLU:OE1	2.42	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:G:21:ASP:O	1:G:24:GLN:HG2	2.03	0.58
1:G:507:LYS:HZ1	1:G:559:MET:CE	2.05	0.58
1:A:431:HIS:CD2	1:A:434:VAL:H	2.22	0.58
1:A:483:ARG:O	1:A:488:ILE:HD11	2.04	0.58
1:F:206:LYS:HD2	1:F:237:PHE:CD1	2.38	0.58
1:E:685:ASN:ND2	1:E:685:ASN:C	2.49	0.58
1:A:472:TRP:CZ2	1:A:476:ARG:HD3	2.39	0.58
1:G:431:HIS:CD2	1:G:434:VAL:H	2.22	0.58
1:E:500:ASN:O	1:E:512:ARG:NH1	2.36	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:C:500:ASN:O	1:C:512:ARG:NH1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:HIS:CD2	1:D:434:VAL:H	2.22	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:H:475:TYR:CZ	1:H:479:LYS:HD3	2.39	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:F:592[B]:MET:SD	1:F:631:MET:HE1	2.44	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:C:745:GLU:OE1	1:C:745:GLU:C	2.43	0.57
1:D:53:MET:CE	1:D:145:ARG:HG2	2.34	0.57
1:H:417:LYS:O	1:H:421:GLU:HG3	2.04	0.57
1:G:448:LEU:HD22	1:G:448:LEU:N	2.19	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:573:ILE:CD1	1:G:574:PHE:N	2.48	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: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:O	1:H:604:ILE:HG23	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: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:C:483:ARG:HB3	1:C:487:GLU:OE2	2.05	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
1:G:503:ASP:CG	1:G:506:SER:HG	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:22:TRP:H	1:H:283:ASN:HD21	1.53	0.56
1:F:320:ASP:C	1:F:320:ASP:OD1	2.44	0.56
1:F:745:GLU:OE1	1:F:745:GLU:C	2.44	0.56
1:H:175:ILE:HG22	1:H:175:ILE:O	2.05	0.56
1:A:709:ASN:HD21	1:A:727:GLY:HA3	1.71	0.56
1:B:109:GLU:HB2	1:E:110:LYS:HZ2	1.69	0.56
1:E:270:ASN:OD1	1:E:273:GLN:HG3	2.06	0.56
1:H:706:MET:CE	1:H:741:ARG:HH22	2.08	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:G:503:ASP:CG	1:G:506:SER:OG	2.43	0.56
1:B:481:LEU:N	1:B:481:LEU:CD1	2.68	0.56
1:H:475:TYR:CD1	1:H:476:ARG:N	2.74	0.56
1:H:480:GLU:C	1:H:481:LEU:HD23	2.26	0.56
1:G:320:ASP:OD1	1:G:320:ASP:C	2.44	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: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:G:443:GLU:CD	1:G:443:GLU:H	2.10	0.55
1:B:547:PRO:HB2	1:B:613:TYR:CD2	2.42	0.55
1:F:680:THR:C	1:F:681:LEU:HD23	2.27	0.55
1:G:336:LEU:HB3	1:G:337:PRO:HD2	1.88	0.55
1:C:592[B]:MET:CE	1:C:631:MET:HE2	2.27	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:G:515:ASP:OD1	1:G:515:ASP:C	2.44	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:F:721:GLU:CD	1:F:721:GLU:N	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:GLU:HA	1:C:442:TYR:CD2	2.42	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:A:320:ASP:C	1:A:320:ASP:OD1	2.44	0.55
1:A:348:ASP:OD1	3:A:801:SWA:O1	2.12	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:D:375:THR:O	1:D:379:SER:OG	2.12	0.54
1:E:503:ASP:OD2	1:E:506:SER:OG	2.25	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:565:ASP:OD2	1:H:619:LYS:NZ	2.41	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:B:455:VAL:O	1:B:456:LYS:HB2	2.07	0.54
1:C:738:ASN:C	1:C:738:ASN:OD1	2.46	0.54
1:B:503:ASP:OD2	1:B:506:SER:OG	2.25	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:H:443:GLU:CD	1:H:443:GLU:N	2.60	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: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: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:HG22	1:G:175:ILE:O	2.07	0.54
1:G:663:CYS:O	1:G:666:THR:HG23	2.07	0.54
1:C:546:ASP:CG	1:C:753:SER:OG	2.45	0.54
1:C:565:ASP:OD2	1:C:619:LYS:NZ	2.40	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:B:320:ASP:OD1	1:B:320:ASP:C	2.46	0.53
1:E:421:GLU:HG2	5:E:2061:HOH:O	2.08	0.53
1:F:721:GLU:CD	1:F:721:GLU:H	2.11	0.53
1:H:592:MET:SD	1:H:631:MET:HE2	2.46	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:F:60:THR:O	1:F:77:ARG:NH1	2.39	0.53
1:F:706:MET:HE2	1:F:741:ARG:NH2	2.23	0.53
1:G:167:ASP:OD1	1:G:167:ASP:C	2.47	0.53
1:B:738:ASN:OD1	1:B:738:ASN:C	2.46	0.53
1:E:176:PRO:HD2	1:E:177:GLU:OE1	2.08	0.53
1:G:53:MET:CE	1:G:145:ARG:HG2	2.39	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:G:738:ASN:C	1:G:738:ASN:OD1	2.47	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:700:ASN:ND2	1:E:735:ASN:HB3	2.23	0.53
1:F:592[B]:MET:SD	1:F:631:MET:CE	2.96	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
1:B:592[B]:MET:HE2	1:B:631:MET:SD	2.42	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

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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	0.53
1:C:564:MET:HE1	1:C:610:LEU:HB2	1.90	0.53
1:D:507:LYS:CE	1:D:559:MET:HE2	2.38	0.53
1:D:588:GLU:O	1:D:592[A]:MET:HG3	2.09	0.53
1:E:680:THR:C	1:E:681:LEU:HD23	2.29	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: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: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:G:502:PHE:C	1:G:502:PHE:CD2	2.81	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:H:515:ASP:OD1	1:H:515:ASP:C	2.48	0.53
1:C:477:LEU:HG	1:C:481:LEU:HD22	1.92	0.52
1:D:570:VAL:CG2	1:D:570:VAL:O	2.56	0.52
1:E:365:ASN:O	1:E:369:GLN:HG2	2.10	0.52
1:E:503:ASP:C	1:E:503:ASP:OD1	2.44	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:475:TYR:CD1	1:H:475:TYR:C	2.82	0.52
1:H:519:GLN:HG2	1:H:520:SER:N	2.23	0.52
1:A:385:TRP:CD1	1:A:393:CYS:HB3	2.44	0.52
1:C:415:ASP:CG	1:C:418:THR:OG1	2.48	0.52
1:C:526:LYS:HA	1:C:575:ASP:HB3	1.90	0.52
1:E:21:ASP:C	1:E:21:ASP:OD1	2.46	0.52
1:F:365:ASN:O	1:F:369:GLN:HG2	2.09	0.52
1:F:564:MET:HE1	1:F:610:LEU:HB2	1.92	0.52
1:G:443:GLU:CD	1:G:443:GLU:N	2.62	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:SER:OG	1:H:318:GLU:CD	2.46	0.52
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:252:SER:OG	1:B:318:GLU:CD	2.45	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:G:750:TYR:C	1:G:750:TYR:CD2	2.83	0.52
1:H:63:MET:HG3	1:H:166:PHE:CE2	2.45	0.52
1:H:555:GLY:C	1:H:559:MET:HE3	2.29	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:350:PHE:C	1:G:350:PHE:CD2	2.83	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:706:MET:CE	1:D:741:ARG:NH2	2.73	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:F:592[B]:MET:HE1	1:F:631:MET:HE1	1.90	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:F:738:ASN:OD1	1:F:738:ASN:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:ASP:CG	1:D:506:SER:OG	2.49	0.51
1:D:507:LYS:HZ2	1:D:559:MET:CE	2.14	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: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
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:D:482:LYS:HE2	5:D:2070:HOH:O	2.11	0.51
1:D:706:MET:HE3	1:D:741:ARG:NH2	2.21	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:G:358:ASN:ND2	1:G:365:ASN:HD22	2.08	0.51
1:H:738:ASN:C	1:H:738:ASN:OD1	2.49	0.51
1:B:153:PHE:CE1	1:B:159:SER:HB3	2.46	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:507:LYS:HZ3	1:A:559:MET:CE	2.07	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:E:455:VAL:O	1:E:456:LYS:HB2	2.10	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:A:363:SER:OG	1:A:684:GLU:CD	2.49	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:B:415:ASP:CG	1:B:418:THR:OG1	2.50	0.50
1:D:175:ILE:O	1:D:175:ILE:HG22	2.11	0.50
1:D:700:ASN:HD22	1:D:735:ASN:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:519:GLN:HG2	1:D:520:SER:N	2.27	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:F:515:ASP:OD1	1:F:515:ASP:C	2.49	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
1:A:663:CYS:O	1:A:666:THR:HG23	2.11	0.50
1:B:175:ILE:HG22	1:B:175:ILE:O	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: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:E:336:LEU:HB3	1:E:337:PRO:HD2	1.93	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:415:ASP:CG	1:H:418:THR:HG1	2.09	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:G:706:MET:HE2	1:G:741:ARG:NH2	2.27	0.50
1:H:365:ASN:O	1:H:368:MET:N	2.45	0.50
1:A:53:MET:CE	1:A:145:ARG:HG2	2.42	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:D:738:ASN:OD1	1:D:738:ASN:C	2.49	0.50
1:F:407:TYR:CE2	1:F:412:LYS:HD3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:459:GLU:O	1:E:463:ARG:HG3	2.12	0.49
1:H:431:HIS:HD2	1:H:434:VAL:H	1.61	0.49
1:A:507:LYS:NZ	1:A:554:MET:O	2.45	0.49
1:C:415:ASP:CG	1:C:418:THR:HG1	2.16	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:D:750:TYR:C	1:D:750:TYR:CD2	2.85	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: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: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:503:ASP:OD2	1:A:506:SER:OG	2.30	0.49
1:C:320:ASP:OD1	1:C:320:ASP:C	2.49	0.49
1:C:555:GLY:O	1:C:559:MET:HG3	2.13	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: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:G:550:LEU:C	1:G:553:LEU:CD2	2.78	0.49
1:H:455:VAL:O	1:H:456:LYS:HB2	2.12	0.49
1:A:738:ASN:OD1	1:A:738:ASN:C	2.51	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:O	1:A:604:ILE:HG23	2.13	0.49
1:B:367:GLU:OE2	4:B:804:GOL:H31	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:738:ASN:C	1:E:738:ASN:OD1	2.50	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:D:706:MET:CE	1:D:741:ARG:HH22	2.24	0.48
1:E:320:ASP:OD1	1:E:320:ASP:C	2.52	0.48
1:E:459:GLU:HG2	1:E:531:PHE:O	2.13	0.48
1:E:503:ASP:CG	1:E:506:SER:OG	2.51	0.48
1:E:515:ASP:OD1	1:E:517:THR:OG1	2.27	0.48
1:G:616:GLN:HG2	1:G:618:TRP:CH2	2.49	0.48
1:B:592[B]:MET:HE1	1:B:631:MET:HE2	1.74	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: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:O	1:G:419:LEU:HD12	2.13	0.48
1:H:700:ASN:ND2	1:H:735:ASN:HB3	2.28	0.48
1:F:448:LEU:N	1:F:448:LEU:HD22	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:B:503:ASP:CG	1:B:506:SER:OG	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:607:MET:O	1:C:610:LEU:HB2	2.14	0.48
1:F:332:ASN:OD1	1:F:332:ASN:C	2.52	0.48
1:F:461:ALA:HB3	1:F:530:ALA:O	2.14	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
1:D:507:LYS:NZ	1:D:559:MET:HE1	2.20	0.48
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:H:750:TYR:C	1:H:750:TYR:CD2	2.86	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: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:E:616:GLN:HG2	1:E:618:TRP:CZ2	2.48	0.47
1:H:350:PHE:CD2	1:H:351:ARG:N	2.82	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:F:750:TYR:C	1:F:750:TYR:CD2	2.87	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:GLU:HG3	4:D:802:GOL:C3	2.40	0.47
1:E:517:THR:H	1:E:517:THR:HG1	1.48	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
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: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:B:706:MET:HE2	1:B:741:ARG:NH2	2.28	0.47
1:C:293:GLY:HA3	1:C:677:LYS:HB2	1.97	0.47
1:C:515:ASP:OD1	1:C:517:THR:OG1	2.30	0.47
1:D:320:ASP:OD1	1:D:320:ASP:C	2.52	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:G:564:MET:HE1	1:G:610:LEU:CB	2.43	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:O	1:A:175:ILE:HG22	2.15	0.47
1:A:358:ASN:HD21	1:A:365:ASN:ND2	2.13	0.47
1:A:611:TYR:HB2	1:A:620:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:209:THR:O	1:C:209:THR:CG2	2.62	0.47
1:D:53:MET:HE2	1:D:145:ARG:HG2	1.97	0.47
1:A:477:LEU:HG	1:A:481:LEU:HD22	1.96	0.47
1:B:483:ARG:HB3	1:B:487:GLU:OE2	2.15	0.47
1:B:507:LYS:CE	1:B:559[B]:MET:HE2	2.45	0.47
1:E:167:ASP:O	1:E:168:LYS:HB2	2.14	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: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: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:N	1:C:681:LEU:HD23	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:E:750:TYR:C	1:E:750:TYR:CD2	2.88	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:H:592:MET:CE	1:H:592:MET:CA	2.90	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: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:B:627:VAL:HG13	1:B:631:MET:HG3	1.96	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:362:PRO:HD2	1:E:684:GLU:CD	2.36	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:A:20:LYS:HD2	1:A:20:LYS:C	2.35	0.46
1:B:153:PHE:CD1	1:B:159:SER:HB3	2.51	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: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: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: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: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: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:257[A]:GLU:H	1:E:257[A]:GLU:CD	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:H:623:TRP:O	1:H:626:GLN:HB2	2.15	0.45
1:B:353:LEU:C	1:B:353:LEU:HD13	2.36	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: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:A:583:ILE:HD12	1:A:585:GLU:HG2	1.98	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:G:526:LYS:O	1:G:535:ASN:HB3	2.17	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:A:515:ASP:OD1	1:A:517:THR:OG1	2.30	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
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:A:29:LEU:HD23	1:A:45:PRO:HG3	1.98	0.45
1:A:558[B]:GLU:H	1:A:558[B]:GLU:CD	2.18	0.45
1:C:680:THR:C	1:C:681:LEU:HD23	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:558[A]:GLU:CD	1:B:558[A]:GLU:H	2.19	0.45
1:H:564:MET:HE3	1:H:610:LEU:HB3	1.99	0.45
1:A:705:SER:OG	1:A:732[A]:ASP:OD2	2.30	0.45
1:B:90:ASN:HB3	1:B:189:SER:OG	2.17	0.45
1:B:706:MET:HE2	1:B:706:MET:HB2	1.85	0.45
1:C:350:PHE:CD2	1:C:350:PHE:C	2.90	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:F:592[B]:MET:HE2	1:F:592[B]:MET:HB3	1.73	0.45
1:H:141:THR:C	1:H:147:VAL:HG23	2.37	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:D:487:GLU:CD	5:D:2074:HOH:O	2.56	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:A:363:SER:OG	1:A:684:GLU:OE1	2.35	0.44
1:D:288:LYS:NZ	4:D:804:GOL:H31	2.32	0.44
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:A:680:THR:C	1:A:681:LEU:HD23	2.37	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: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
1:A:750:TYR:C	1:A:750:TYR:CD2	2.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
1:E:604:ILE:O	1:E:604:ILE:HG23	2.17	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:A:706:MET:HE2	1:A:741:ARG:NH2	2.33	0.43
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: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: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:209:THR:O	1:F:209:THR:HG22	2.17	0.43
1:F:240:ARG:HB2	1:F:240:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:498:TYR:OH	1:E:546:ASP:OD2	2.29	0.43
1:E:528:GLY:O	1:E:529:ASP:CB	2.66	0.43
1:F:477:LEU:HG	1:F:481:LEU:HD22	2.00	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:N	1:A:481:LEU:HD13	2.34	0.43
1:C:519:GLN:OE1	1:C:521:PRO:O	2.36	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
1:E:706:MET:HE2	1:E:741:ARG:NH2	2.30	0.43
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:HG22	1:C:175:ILE:O	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:F:517:THR:H	1:F:517:THR:HG1	1.54	0.43
1:G:332:ASN:C	1:G:332:ASN:OD1	2.57	0.43
1:G:553:LEU:HD22	1:G:553:LEU:N	2.27	0.43
1:G:706:MET:HE2	1:G:706:MET:HB2	1.89	0.43
1:E:570:VAL:HG23	1:E:571:PRO:O	2.19	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: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:G:558:GLU:CD	1:G:558:GLU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:519:GLN:HG2	1:B:520:SER:N	2.34	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:H:502:PHE:CD2	1:H:502:PHE:C	2.92	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:HB2	1:C:240:ARG:NH1	2.34	0.43
1:G:199:TYR:O	1:G:251:SER:HA	2.19	0.43
1:G:507:LYS:NZ	1:G:559:MET:HE3	2.14	0.43
1:H:92:TYR:OH	1:H:343:ASP:OD2	2.22	0.43
1:H:397:ASN:HD22	1:H:439:ARG:NE	2.04	0.43
1:B:507:LYS:NZ	1:B:559[B]:MET:CE	2.82	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:616:GLN:HG2	1:H:618:TRP:CZ2	2.53	0.43
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:507:LYS:HE3	1:D:559:MET:HE2	2.00	0.42
1:D:515:ASP:CG	1:D:517:THR:HG1	2.21	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:H:497:ASN:C	1:H:499:LYS:N	2.69	0.42
1:A:481:LEU:N	1:A:481:LEU:CD1	2.81	0.42
1:B:315:LYS:HZ3	4:B:804:GOL:H32	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:592[B]:MET:SD	1:C:631:MET:CE	3.05	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:HA	1:A:268:LYS:HD3	1.82	0.42
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:84:GLN:HG3	1:B:90:ASN:C	2.40	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:F:592[A]:MET:HE2	1:F:640:CYS:HB2	2.02	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: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:H:706:MET:HE2	1:H:741:ARG:NH2	2.35	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:G:507:LYS:HZ2	1:G:559:MET:HE1	0.63	0.42
1:H:365:ASN:HA	1:H:368:MET:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:754:LYS:C	1:C:756:LEU:H	2.22	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: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:A:332:ASN:OD1	1:A:332:ASN:C	2.58	0.42
1:B:168:LYS:HA	1:B:168:LYS:HD3	1.71	0.42
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:F:706:MET:HE2	1:F:706:MET:HB2	1.86	0.42
1:G:442:TYR:CZ	1:G:443:GLU:CD	2.86	0.42
1:G:483:ARG:HH21	1:G:487:GLU:CD	2.23	0.42
1:H:240:ARG:O	1:H:241:LYS:C	2.58	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: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:C:588:GLU:O	1:C:592[A]:MET:CE	2.68	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:HA	1:G:168:LYS:HD3	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:750:TYR:CD2	1:B:750:TYR:C	2.92	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:G:717:TYR:C	1:G:718:LEU:HD23	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:210:TYR:CD1	1:A:210:TYR:C	2.93	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:C:105:VAL:O	1:C:105:VAL:HG23	2.18	0.41
1:D:59:GLN:HE21	1:D:80:LYS:HB2	1.84	0.41
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: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:553:LEU:H	1:H:553:LEU:HG	1.60	0.41
1:C:564:MET:HE3	1:C:610:LEU:HB3	2.01	0.41
1:C:706:MET:HE2	1:C:741:ARG:NH2	2.35	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:A:517:THR:H	1:A:517:THR:HG1	1.47	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:G:507:LYS:NZ	1:G:554:MET:O	2.51	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:519:GLN:OE1	1:B:521:PRO:O	2.38	0.41
1:B:680:THR:C	1:B:681:LEU:HD23	2.41	0.41
1:D:88:TRP:HB2	3:D:801:SWA:HC62	2.01	0.41
1:D:623:TRP:O	1:D:626:GLN:HB2	2.20	0.41
1:E:350:PHE:CD2	1:E:350:PHE:C	2.94	0.41
1:E:448:LEU:N	1:E:448:LEU:HD22	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:H:293:GLY:HA3	1:H:677:LYS:HB2	2.02	0.41
1:H:398:ASN:O	1:H:399:SER:C	2.57	0.41
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:H:398:ASN:C	1:H:400:ALA:N	2.72	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:N	1:C:448:LEU:HD22	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:481:LEU:HA	1:F:481:LEU:HD12	1.89	0.41
1:F:592[B]:MET:CE	1:F:631:MET:CE	2.87	0.41
1:G:177:GLU:CD	1:G:177:GLU:H	2.24	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:442:TYR:CE1	1:H:443:GLU:CD	2.93	0.41
1:H:452:PRO:HB2	1:H:455:VAL:HG22	2.01	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:C:706:MET:HE2	1:C:706:MET:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:483:ARG:HH21	1:F:487:GLU:CD	2.24	0.41
1:G:456:LYS:HD2	1:G:456:LYS:HA	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:592[B]:MET:HE2	1:B:631:MET:HE1	0.45	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
1:E:612:ASP:OD2	1:E:671:MET:O	2.39	0.40
1:F:717:TYR:C	1:F:718:LEU:HD23	2.41	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: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:503:ASP:C	1:A:503:ASP:OD1	2.59	0.40
1:A:586:ILE:O	1:A:590:THR:HG23	2.21	0.40
1:D:316:PHE:CE2	1:D:330:PRO:HG3	2.56	0.40
1:D:385:TRP:CD1	1:D:393:CYS:HB3	2.56	0.40
1:E:177:GLU:CD	1:E:177:GLU:H	2.25	0.40
1:E:361:TYR:N	1:E:362:PRO:HD3	2.37	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:483:ARG:HH21	1:A:487:GLU:CD	2.25	0.40
1:A:681:LEU:HD23	1:A:681:LEU:N	2.35	0.40
1:B:564:MET:HE1	1:B:610:LEU:CB	2.44	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:442:TYR:CD1	1:G:443:GLU:CD	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:288:LYS:HZ1	4:D:804:GOL:H31	1.87	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
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: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:D:745:GLU:OE1	1:D:745:GLU:C	2.60	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:452:PRO:HB2	1:F:455:VAL:HG13	2.04	0.40
1:H:717:TYR:C	1:H:718:LEU:HD23	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	737/744 (99%)	713 (97%)	22 (3%)	2 (0%)	41 72
1	B	739/744 (99%)	711 (96%)	26 (4%)	2 (0%)	41 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	737/744 (99%)	712 (97%)	23 (3%)	2 (0%)	41	72
1	D	738/744 (99%)	710 (96%)	26 (4%)	2 (0%)	41	72
1	E	736/744 (99%)	711 (97%)	23 (3%)	2 (0%)	41	72
1	F	735/744 (99%)	709 (96%)	23 (3%)	3 (0%)	34	66
1	G	734/744 (99%)	707 (96%)	25 (3%)	2 (0%)	41	72
1	H	734/744 (99%)	707 (96%)	25 (3%)	2 (0%)	41	72
All	All	5890/5952 (99%)	5680 (96%)	193 (3%)	17 (0%)	41	72

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 (i)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	636/643 (99%)	598 (94%)	38 (6%)	19	48
1	B	640/643 (100%)	609 (95%)	31 (5%)	25	58
1	C	636/643 (99%)	599 (94%)	37 (6%)	20	50
1	D	636/643 (99%)	602 (95%)	34 (5%)	22	54
1	E	631/643 (98%)	595 (94%)	36 (6%)	20	50
1	F	631/643 (98%)	595 (94%)	36 (6%)	20	50
1	G	626/643 (97%)	594 (95%)	32 (5%)	24	55
1	H	618/643 (96%)	581 (94%)	37 (6%)	19	48
All	All	5054/5144 (98%)	4773 (94%)	281 (6%)	21	51

All (281) 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	216	ASN
1	A	220	GLN
1	A	237	PHE
1	A	284	GLN
1	A	307	TYR
1	A	319	LEU
1	A	363	SER
1	A	385	TRP
1	A	456	LYS
1	A	460	ASN
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	539	TYR
1	A	553	LEU
1	A	559	MET

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Mol	Chain	Res	Type
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	708	PHE
1	A	714	THR
1	A	719	ARG
1	A	730	LYS
1	A	732[A]	ASP
1	A	732[B]	ASP
1	A	739	LEU
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
1	B	307	TYR
1	B	319	LEU
1	B	363	SER
1	B	385	TRP
1	B	456	LYS
1	B	481	LEU
1	B	486	LYS
1	B	517	THR
1	B	519	GLN
1	B	539	TYR
1	B	553	LEU
1	B	564	MET
1	B	573	ILE
1	B	585	GLU
1	B	610	LEU
1	B	624	LEU
1	B	685	ASN
1	B	689	LEU
1	B	692	ASP
1	B	708	PHE
1	B	714	THR

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Mol	Chain	Res	Type
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	206	LYS
1	C	220	GLN
1	C	237	PHE
1	C	284	GLN
1	C	307	TYR
1	C	319	LEU
1	C	363	SER
1	C	385	TRP
1	C	460	ASN
1	C	475	TYR
1	C	481	LEU
1	C	486	LYS
1	C	517	THR
1	C	519	GLN
1	C	539	TYR
1	C	553	LEU
1	C	564	MET
1	C	573	ILE
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	708	PHE
1	C	714	THR
1	C	730	LYS
1	C	732[A]	ASP
1	C	732[B]	ASP
1	C	736	ARG
1	C	739	LEU
1	C	753	SER
1	C	756	LEU
1	D	77	ARG
1	D	101	VAL

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Mol	Chain	Res	Type
1	D	177	GLU
1	D	206	LYS
1	D	220	GLN
1	D	237	PHE
1	D	284	GLN
1	D	307	TYR
1	D	319	LEU
1	D	363	SER
1	D	385	TRP
1	D	433	GLU
1	D	443	GLU
1	D	448	LEU
1	D	481	LEU
1	D	485	LYS
1	D	519	GLN
1	D	539	TYR
1	D	553	LEU
1	D	558	GLU
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	708	PHE
1	D	714	THR
1	D	719	ARG
1	D	736	ARG
1	D	739	LEU
1	E	77	ARG
1	E	101	VAL
1	E	177	GLU
1	E	206	LYS
1	E	220	GLN
1	E	237	PHE
1	E	284	GLN
1	E	307	TYR
1	E	319	LEU
1	E	363	SER

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Mol	Chain	Res	Type
1	E	385	TRP
1	E	428	GLU
1	E	460	ASN
1	E	475	TYR
1	E	481	LEU
1	E	486	LYS
1	E	517	THR
1	E	519	GLN
1	E	539	TYR
1	E	553	LEU
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
1	E	689	LEU
1	E	692	ASP
1	E	708	PHE
1	E	714	THR
1	E	719	ARG
1	E	730	LYS
1	E	739	LEU
1	E	755	GLU
1	F	77	ARG
1	F	101	VAL
1	F	206	LYS
1	F	220	GLN
1	F	237	PHE
1	F	284	GLN
1	F	307	TYR
1	F	319	LEU
1	F	349	THR
1	F	350	PHE
1	F	363	SER
1	F	385	TRP
1	F	456	LYS
1	F	460	ASN
1	F	481	LEU
1	F	505	GLU

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Mol	Chain	Res	Type
1	F	517	THR
1	F	519	GLN
1	F	539	TYR
1	F	553	LEU
1	F	558	GLU
1	F	564	MET
1	F	573	ILE
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	708	PHE
1	F	714	THR
1	F	730	LYS
1	F	739	LEU
1	F	753	SER
1	F	755	GLU
1	G	77	ARG
1	G	101	VAL
1	G	177	GLU
1	G	206	LYS
1	G	220	GLN
1	G	237	PHE
1	G	284	GLN
1	G	307	TYR
1	G	319	LEU
1	G	363	SER
1	G	385	TRP
1	G	443	GLU
1	G	460	ASN
1	G	481	LEU
1	G	504	LYS
1	G	505	GLU
1	G	517	THR
1	G	519	GLN
1	G	539	TYR
1	G	553	LEU
1	G	573	ILE
1	G	585	GLU

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Mol	Chain	Res	Type
1	G	596	ASN
1	G	610	LEU
1	G	624	LEU
1	G	685	ASN
1	G	689	LEU
1	G	692	ASP
1	G	708	PHE
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	307	TYR
1	H	319	LEU
1	H	350	PHE
1	H	352	CYS
1	H	363	SER
1	H	385	TRP
1	H	433	GLU
1	H	443	GLU
1	H	460	ASN
1	H	475	TYR
1	H	476	ARG
1	H	479	LYS
1	H	517	THR
1	H	519	GLN
1	H	539	TYR
1	H	553	LEU
1	H	573	ILE
1	H	585	GLU
1	H	596	ASN
1	H	610	LEU
1	H	624	LEU
1	H	685	ASN
1	H	692	ASP
1	H	708	PHE

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Mol	Chain	Res	Type
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 (176) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	188	ASN
1	A	216	ASN
1	A	220	GLN
1	A	226	GLN
1	A	264	ASN
1	A	283	ASN
1	A	298	GLN
1	A	358	ASN
1	A	374	ASN
1	A	397	ASN
1	A	431	HIS
1	A	446	ASN
1	A	497	ASN
1	A	500	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	188	ASN
1	B	216	ASN
1	B	220	GLN
1	B	226	GLN
1	B	264	ASN
1	B	283	ASN
1	B	358	ASN
1	B	374	ASN
1	B	397	ASN

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Mol	Chain	Res	Type
1	B	431	HIS
1	B	446	ASN
1	B	497	ASN
1	B	500	ASN
1	B	519	GLN
1	B	581	GLN
1	B	593	ASN
1	B	599	HIS
1	B	685	ASN
1	B	700	ASN
1	B	709	ASN
1	B	716	ASN
1	C	59	GLN
1	C	188	ASN
1	C	216	ASN
1	C	220	GLN
1	C	226	GLN
1	C	264	ASN
1	C	283	ASN
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	497	ASN
1	C	500	ASN
1	C	519	GLN
1	C	593	ASN
1	C	599	HIS
1	C	685	ASN
1	C	700	ASN
1	C	709	ASN
1	D	59	GLN
1	D	158	HIS
1	D	188	ASN
1	D	216	ASN
1	D	226	GLN
1	D	264	ASN
1	D	283	ASN
1	D	358	ASN
1	D	374	ASN

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Mol	Chain	Res	Type
1	D	397	ASN
1	D	431	HIS
1	D	446	ASN
1	D	460	ASN
1	D	497	ASN
1	D	500	ASN
1	D	519	GLN
1	D	593	ASN
1	D	599	HIS
1	D	685	ASN
1	D	695	ASN
1	D	700	ASN
1	D	709	ASN
1	D	713	HIS
1	E	59	GLN
1	E	188	ASN
1	E	226	GLN
1	E	264	ASN
1	E	283	ASN
1	E	358	ASN
1	E	374	ASN
1	E	397	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	599	HIS
1	E	685	ASN
1	E	695	ASN
1	E	700	ASN
1	E	709	ASN
1	E	713	HIS
1	F	59	GLN
1	F	188	ASN
1	F	216	ASN
1	F	220	GLN
1	F	226	GLN
1	F	264	ASN
1	F	283	ASN

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Mol	Chain	Res	Type
1	F	358	ASN
1	F	374	ASN
1	F	397	ASN
1	F	398	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	599	HIS
1	F	685	ASN
1	F	700	ASN
1	F	709	ASN
1	G	59	GLN
1	G	188	ASN
1	G	216	ASN
1	G	220	GLN
1	G	226	GLN
1	G	264	ASN
1	G	283	ASN
1	G	358	ASN
1	G	374	ASN
1	G	397	ASN
1	G	431	HIS
1	G	446	ASN
1	G	460	ASN
1	G	497	ASN
1	G	500	ASN
1	G	519	GLN
1	G	593	ASN
1	G	599	HIS
1	G	685	ASN
1	G	695	ASN
1	G	700	ASN
1	G	709	ASN
1	H	59	GLN
1	H	188	ASN
1	H	216	ASN
1	H	220	GLN
1	H	226	GLN

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Mol	Chain	Res	Type
1	H	264	ASN
1	H	283	ASN
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	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
3	SWA	B	801	2	13,13,13	1.08	2 (15%)	13,19,19	1.89	3 (23%)
4	GOL	F	802	-	5,5,5	0.38	0	5,5,5	0.45	0
4	GOL	A	804	-	5,5,5	0.56	0	5,5,5	1.28	1 (20%)
3	SWA	F	801	2	13,13,13	0.73	0	13,19,19	0.91	0
4	GOL	B	802	-	5,5,5	0.37	0	5,5,5	0.67	0
4	GOL	E	803	-	5,5,5	0.40	0	5,5,5	0.41	0
4	GOL	B	803	-	5,5,5	0.43	0	5,5,5	0.55	0
4	GOL	B	804	-	5,5,5	0.47	0	5,5,5	1.04	0
3	SWA	A	801	2	13,13,13	0.64	0	13,19,19	2.54	1 (7%)
3	SWA	D	801	2	13,13,13	1.33	2 (15%)	13,19,19	2.34	3 (23%)
4	GOL	C	802	-	5,5,5	0.42	0	5,5,5	0.24	0
4	GOL	C	804	-	5,5,5	0.41	0	5,5,5	1.14	1 (20%)
4	GOL	A	806	-	5,5,5	0.42	0	5,5,5	0.31	0
4	GOL	D	804	-	5,5,5	0.40	0	5,5,5	0.54	0
4	GOL	E	802	-	5,5,5	0.36	0	5,5,5	0.82	0
4	GOL	A	802	-	5,5,5	0.35	0	5,5,5	0.18	0
3	SWA	C	801	2	13,13,13	0.93	0	13,19,19	2.06	4 (30%)
4	GOL	D	802	-	5,5,5	0.40	0	5,5,5	0.23	0
4	GOL	A	803	-	5,5,5	0.45	0	5,5,5	1.24	0
4	GOL	D	803	-	5,5,5	0.40	0	5,5,5	0.89	0
3	SWA	E	801	2	13,13,13	0.83	0	13,19,19	1.99	3 (23%)
4	GOL	A	805	-	5,5,5	0.34	0	5,5,5	0.62	0
3	SWA	G	801	2	13,13,13	1.29	1 (7%)	13,19,19	1.93	2 (15%)
4	GOL	C	803	-	5,5,5	0.47	0	5,5,5	0.57	0
3	SWA	H	801	2	13,13,13	1.18	1 (7%)	13,19,19	2.45	3 (23%)

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
3	SWA	B	801	2	-	-	0/2/2/2
4	GOL	F	802	-	-	2/4/4/4	-
4	GOL	A	804	-	-	2/4/4/4	-
3	SWA	F	801	2	-	-	0/2/2/2
4	GOL	B	802	-	-	0/4/4/4	-
4	GOL	E	803	-	-	3/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	SWA	C2-C1	3.79	1.57	1.52
3	G	801	SWA	C7-C3	3.32	1.58	1.53
3	H	801	SWA	C7-C3	2.48	1.57	1.53
3	B	801	SWA	C8-C7	-2.39	1.49	1.53
3	D	801	SWA	C1-C3	2.21	1.56	1.53
3	B	801	SWA	C1-C3	-2.00	1.50	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	SWA	C5-N4-C3	8.66	120.87	112.14
3	H	801	SWA	C5-N4-C3	6.54	118.73	112.14
3	D	801	SWA	C5-N4-C3	6.47	118.66	112.14
3	E	801	SWA	C5-N4-C3	5.59	117.77	112.14
3	B	801	SWA	C5-N4-C3	4.98	117.16	112.14
3	C	801	SWA	C5-N4-C3	4.68	116.85	112.14
3	H	801	SWA	C5-N4-C9	-4.54	104.48	115.44
3	G	801	SWA	C5-N4-C3	-4.35	107.75	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	801	SWA	C5-N4-C9	-3.85	106.14	115.44
3	D	801	SWA	C2-C1-C3	3.64	117.90	110.71
3	C	801	SWA	C2-C1-C3	3.10	116.83	110.71
3	E	801	SWA	O11-C7-C8	-2.84	105.19	112.04
3	H	801	SWA	C9-N4-C3	-2.70	99.07	104.89
3	C	801	SWA	O11-C7-C8	-2.68	105.58	112.04
3	D	801	SWA	C9-N4-C3	2.66	110.61	104.89
3	C	801	SWA	O13-C8-C7	-2.32	106.86	111.27
3	B	801	SWA	O13-C8-C9	-2.19	105.77	110.94
4	C	804	GOL	O2-C2-C3	2.11	118.41	109.12
3	B	801	SWA	O11-C7-C8	-2.07	107.04	112.04
3	E	801	SWA	C2-C1-C3	2.02	114.70	110.71
4	A	804	GOL	O1-C1-C2	2.00	119.80	110.20

There are no chirality outliers.

All (36) 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	O1-C1-C2-C3
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	A	806	GOL	C1-C2-C3-O3
4	C	803	GOL	O1-C1-C2-C3
4	C	803	GOL	C1-C2-C3-O3
4	C	804	GOL	O1-C1-C2-C3
4	A	802	GOL	O1-C1-C2-O2
4	A	802	GOL	O2-C2-C3-O3
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

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Mol	Chain	Res	Type	Atoms
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	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	E	803	GOL	O1-C1-C2-O2
4	A	804	GOL	O2-C2-C3-O3
4	B	803	GOL	C1-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 50 short contacts:

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

5.7 Other polymers

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, 95^{th} 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%)	-0.31	0 100 100	7, 12, 20, 24	0
1	B	736/744 (98%)	-0.28	0 100 100	7, 12, 20, 25	0
1	C	737/744 (99%)	-0.24	3 (0%) 92 91	7, 12, 20, 29	0
1	D	738/744 (99%)	-0.31	1 (0%) 95 95	7, 12, 20, 36	0
1	E	736/744 (98%)	-0.14	7 (0%) 82 77	7, 12, 19, 26	0
1	F	736/744 (98%)	-0.01	16 (2%) 62 52	7, 12, 19, 24	0
1	G	736/744 (98%)	0.28	36 (4%) 29 20	7, 12, 19, 24	0
1	H	736/744 (98%)	0.54	76 (10%) 6 3	7, 12, 19, 24	0
All	All	5891/5952 (98%)	-0.06	139 (2%) 59 49	7, 12, 19, 36	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	717	TYR	5.8
1	H	723	LEU	5.7
1	H	708	PHE	5.5
1	H	613	TYR	4.7
1	H	681	LEU	4.6
1	H	657	LEU	4.4
1	H	668	GLU	4.4
1	H	718	LEU	4.3
1	G	450	TYR	4.3
1	H	670	VAL	4.1
1	H	720	HIS	4.0
1	H	611	TYR	4.0
1	H	731	VAL	3.7
1	H	364	VAL	3.7
1	H	689	LEU	3.7
1	H	683	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	729	ILE	3.6
1	H	560	PHE	3.5
1	G	448	LEU	3.5
1	H	749	PRO	3.5
1	H	382	PHE	3.5
1	F	441	GLY	3.5
1	H	669	TYR	3.4
1	H	674	PRO	3.4
1	H	659	PHE	3.4
1	H	724	PHE	3.3
1	H	691	ILE	3.3
1	G	669	TYR	3.2
1	H	748	MET	3.2
1	H	721	GLU	3.2
1	F	452	PRO	3.2
1	G	668	GLU	3.2
1	H	706	MET	3.0
1	G	613	TYR	3.0
1	G	493	LYS	3.0
1	H	610	LEU	3.0
1	G	496	MET	3.0
1	H	477	LEU	3.0
1	H	750	TYR	3.0
1	G	474	ILE	2.9
1	H	746	GLU	2.9
1	H	671	MET	2.9
1	H	291	VAL	2.9
1	H	481	LEU	2.9
1	E	216[A]	ASN	2.9
1	E	690	VAL	2.8
1	H	407	TYR	2.8
1	E	691	ILE	2.8
1	E	679	ALA	2.8
1	G	491	PHE	2.8
1	H	703	ILE	2.8
1	F	450	TYR	2.8
1	G	749	PRO	2.7
1	G	407	TYR	2.7
1	F	720	HIS	2.7
1	H	753	SER	2.7
1	H	268	LYS	2.7
1	H	719	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	447	LYS	2.6
1	H	675	LEU	2.6
1	H	614	ALA	2.6
1	G	441	GLY	2.6
1	G	550	LEU	2.6
1	H	475	TYR	2.6
1	H	665	GLY	2.5
1	H	615	GLY	2.5
1	C	448	LEU	2.5
1	G	532	THR	2.5
1	G	461	ALA	2.5
1	H	658	GLY	2.5
1	F	451	VAL	2.5
1	G	689	LEU	2.5
1	G	413	VAL	2.4
1	H	403	LEU	2.4
1	H	207	PRO	2.4
1	H	541	TRP	2.4
1	H	662	VAL	2.4
1	G	172	ILE	2.4
1	G	455	VAL	2.4
1	H	725	LYS	2.4
1	H	660	TYR	2.4
1	F	491	PHE	2.4
1	G	752	PHE	2.4
1	G	516	GLY	2.4
1	H	380	GLY	2.4
1	H	474	ILE	2.4
1	G	665	GLY	2.4
1	F	496	MET	2.4
1	F	446	ASN	2.4
1	G	449	GLY	2.3
1	C	449	GLY	2.3
1	G	544	PHE	2.3
1	G	438	GLY	2.3
1	E	708	PHE	2.3
1	F	473	CYS	2.3
1	F	532	THR	2.3
1	H	742	GLY	2.3
1	H	548	GLN	2.3
1	H	663	CYS	2.3
1	H	609	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	716	ASN	2.3
1	H	618	TRP	2.3
1	H	438	GLY	2.3
1	G	490	LEU	2.3
1	G	670	VAL	2.2
1	H	439	ARG	2.2
1	H	714	THR	2.2
1	E	689	LEU	2.2
1	G	440	LEU	2.2
1	H	476	ARG	2.2
1	H	667	ASP	2.2
1	H	617	PRO	2.2
1	E	449	GLY	2.2
1	D	569	ALA	2.2
1	H	666	THR	2.2
1	H	558	GLU	2.2
1	F	723	LEU	2.2
1	G	513	ASN	2.2
1	H	472	TRP	2.1
1	C	450	TYR	2.1
1	G	664	PRO	2.1
1	H	557	LYS	2.1
1	F	445	TYR	2.1
1	F	543	VAL	2.1
1	F	448	LEU	2.1
1	H	413	VAL	2.1
1	H	554	MET	2.1
1	G	444	TYR	2.1
1	H	400	ALA	2.1
1	H	620	ALA	2.1
1	F	721	GLU	2.1
1	G	160	TYR	2.0
1	G	286	LEU	2.0
1	H	606	HIS	2.0
1	F	669	TYR	2.0
1	H	711	ALA	2.0
1	H	420	TYR	2.0
1	G	418	THR	2.0
1	G	452	PRO	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 monosaccharides 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, 95^{th} 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	0.66	0.34	59,60,60,61	0
3	SWA	H	801	12/12	0.79	0.23	25,27,30,33	0
4	GOL	C	803	6/6	0.81	0.27	32,33,34,34	0
4	GOL	C	804	6/6	0.83	0.34	32,33,33,35	0
4	GOL	A	804	6/6	0.87	0.25	19,19,21,22	0
3	SWA	G	801	12/12	0.87	0.23	39,40,42,45	0
2	CA	H	800	1/1	0.88	0.10	43,43,43,43	0
4	GOL	E	803	6/6	0.88	0.21	38,39,39,39	0
4	GOL	D	804	6/6	0.89	0.30	29,30,31,34	0
4	GOL	B	804	6/6	0.89	0.19	22,26,26,28	0
4	GOL	A	806	6/6	0.91	0.18	42,43,44,45	0
4	GOL	D	802	6/6	0.92	0.34	30,33,34,36	0
4	GOL	B	802	6/6	0.93	0.29	29,30,30,31	0
2	CA	E	800	1/1	0.93	0.06	33,33,33,33	0
4	GOL	A	802	6/6	0.94	0.24	42,43,44,45	0
2	CA	F	800	1/1	0.94	0.07	22,22,22,22	0
4	GOL	A	805	6/6	0.94	0.19	31,33,34,34	0
3	SWA	F	801	12/12	0.95	0.21	22,24,24,25	0
2	CA	D	800	1/1	0.95	0.05	30,30,30,30	0
3	SWA	A	801	12/12	0.95	0.18	37,39,40,41	0
3	SWA	D	801	12/12	0.95	0.14	17,18,20,21	0
4	GOL	D	803	6/6	0.95	0.29	32,33,35,35	0
4	GOL	B	803	6/6	0.95	0.18	45,45,46,47	0
4	GOL	E	802	6/6	0.95	0.16	30,31,31,31	0
4	GOL	A	803	6/6	0.95	0.21	32,35,35,36	0
4	GOL	F	802	6/6	0.95	0.18	30,32,33,33	0
3	SWA	E	801	12/12	0.96	0.12	8,11,13,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	A	800	1/1	0.96	0.07	28,28,28,28	0
2	CA	C	800	1/1	0.96	0.06	23,23,23,23	0
3	SWA	C	801	12/12	0.97	0.23	18,21,22,24	0
3	SWA	B	801	12/12	0.98	0.13	9,14,15,17	0
2	CA	G	800	1/1	0.98	0.14	39,39,39,39	0
2	CA	B	800	1/1	0.99	0.07	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.