



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:17 PM BST

PDB ID : 1XSK
Title : Structure of a Family 31 alpha glycosidase glycosyl-enzyme intermediate
Authors : Lovering, A.L.; Lee, S.S.; Kim, Y.W.; Withers, S.G.; Strynadka, N.C.
Deposited on : 2004-10-19
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

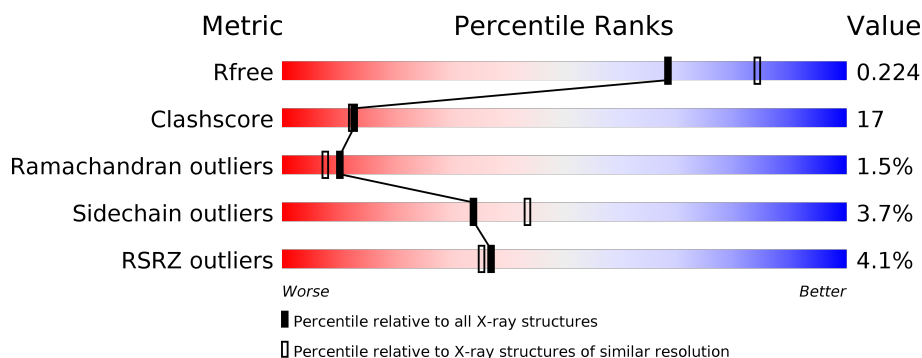
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	778	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>..</div> </div> </div>
1	B	778	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>30%</div> <div>..</div> </div> </div>
1	C	778	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div>..</div> </div> </div>
1	D	778	<div> <div>7%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>..</div> </div> </div>
1	E	778	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>..</div> </div> </div>
1	F	778	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>..</div> </div> </div>

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
2	SO4	F	3005	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38360 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 family 31 glucosidase yicI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	B	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	C	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	D	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	E	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	F	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	773	HIS	-	expression tag	UNP P31434
A	774	HIS	-	expression tag	UNP P31434
A	775	HIS	-	expression tag	UNP P31434
A	776	HIS	-	expression tag	UNP P31434
A	777	HIS	-	expression tag	UNP P31434
A	778	HIS	-	expression tag	UNP P31434
B	773	HIS	-	expression tag	UNP P31434
B	774	HIS	-	expression tag	UNP P31434
B	775	HIS	-	expression tag	UNP P31434
B	776	HIS	-	expression tag	UNP P31434
B	777	HIS	-	expression tag	UNP P31434
B	778	HIS	-	expression tag	UNP P31434
C	773	HIS	-	expression tag	UNP P31434
C	774	HIS	-	expression tag	UNP P31434
C	775	HIS	-	expression tag	UNP P31434
C	776	HIS	-	expression tag	UNP P31434
C	777	HIS	-	expression tag	UNP P31434

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Chain	Residue	Modelled	Actual	Comment	Reference
C	778	HIS	-	expression tag	UNP P31434
D	773	HIS	-	expression tag	UNP P31434
D	774	HIS	-	expression tag	UNP P31434
D	775	HIS	-	expression tag	UNP P31434
D	776	HIS	-	expression tag	UNP P31434
D	777	HIS	-	expression tag	UNP P31434
D	778	HIS	-	expression tag	UNP P31434
E	773	HIS	-	expression tag	UNP P31434
E	774	HIS	-	expression tag	UNP P31434
E	775	HIS	-	expression tag	UNP P31434
E	776	HIS	-	expression tag	UNP P31434
E	777	HIS	-	expression tag	UNP P31434
E	778	HIS	-	expression tag	UNP P31434
F	773	HIS	-	expression tag	UNP P31434
F	774	HIS	-	expression tag	UNP P31434
F	775	HIS	-	expression tag	UNP P31434
F	776	HIS	-	expression tag	UNP P31434
F	777	HIS	-	expression tag	UNP P31434
F	778	HIS	-	expression tag	UNP P31434

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



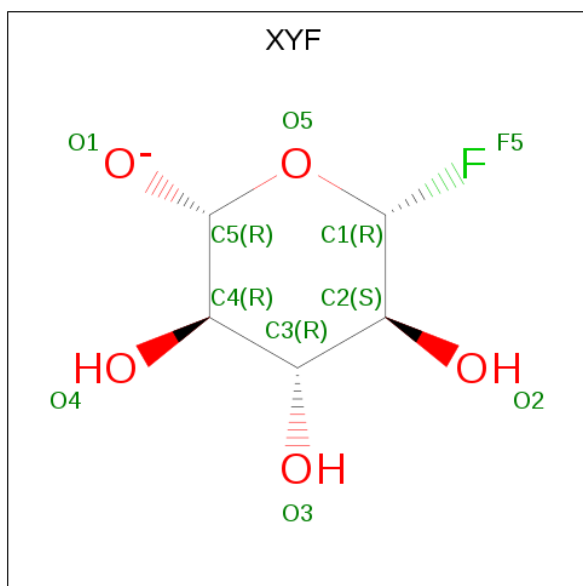
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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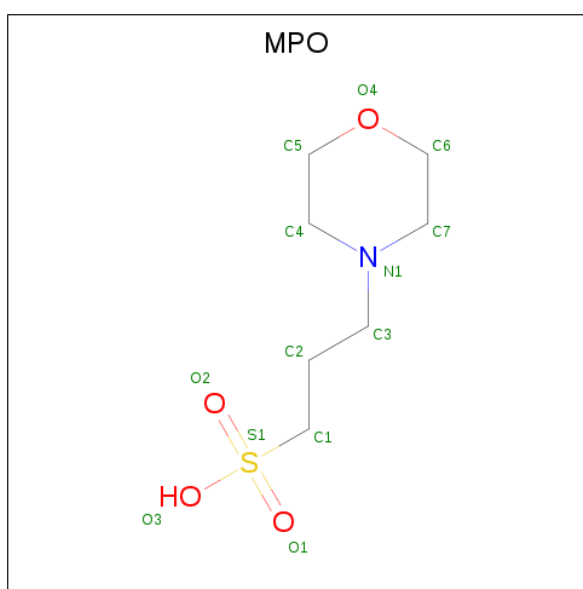
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 5(R)-fluoro-beta-D-xylopyranose (three-letter code: XYF) (formula: C₅H₈FO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			10	5	1	4		
3	B	1	Total	C	F	O	0	0
			10	5	1	4		
3	C	1	Total	C	F	O	0	0
			10	5	1	4		
3	E	1	Total	C	F	O	0	0
			10	5	1	4		

- Molecule 4 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C₇H₁₅NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	E	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

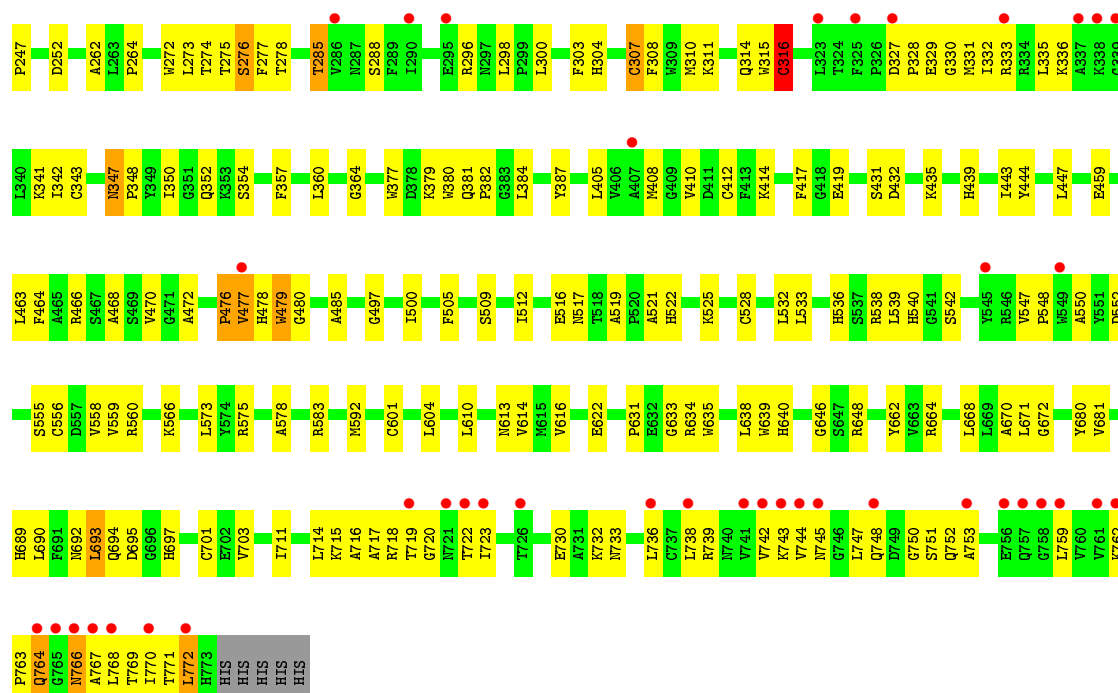
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	168	Total	O	0	0
			168	168		

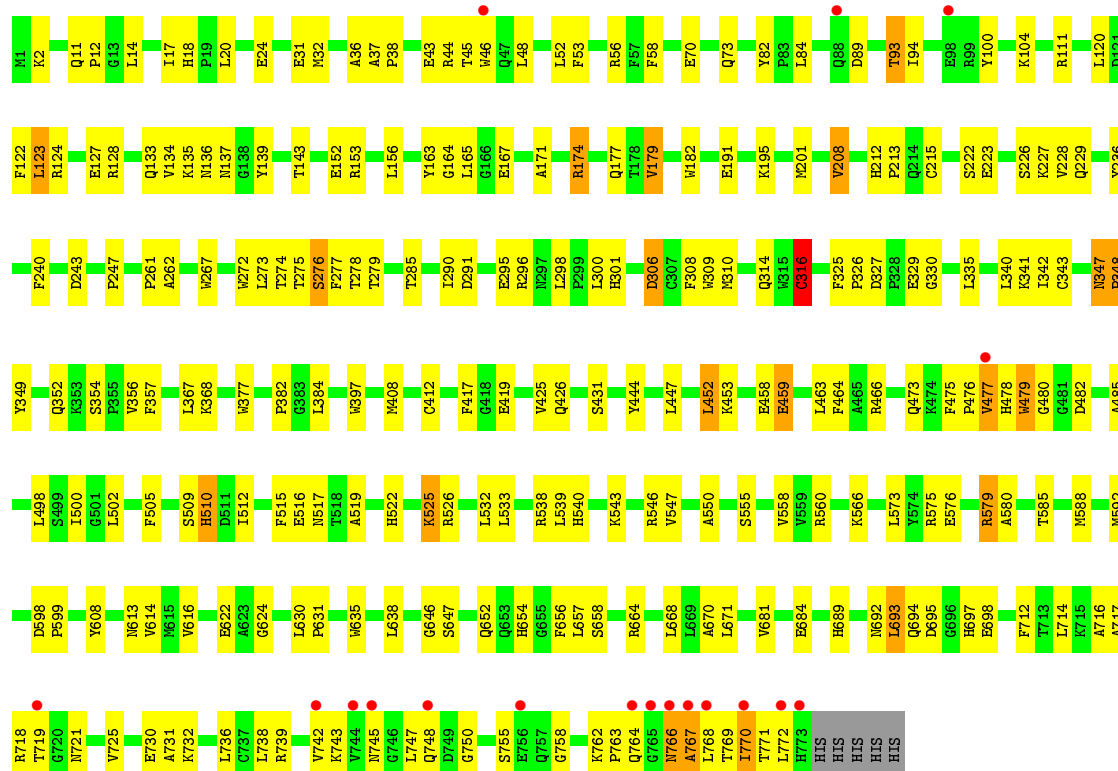
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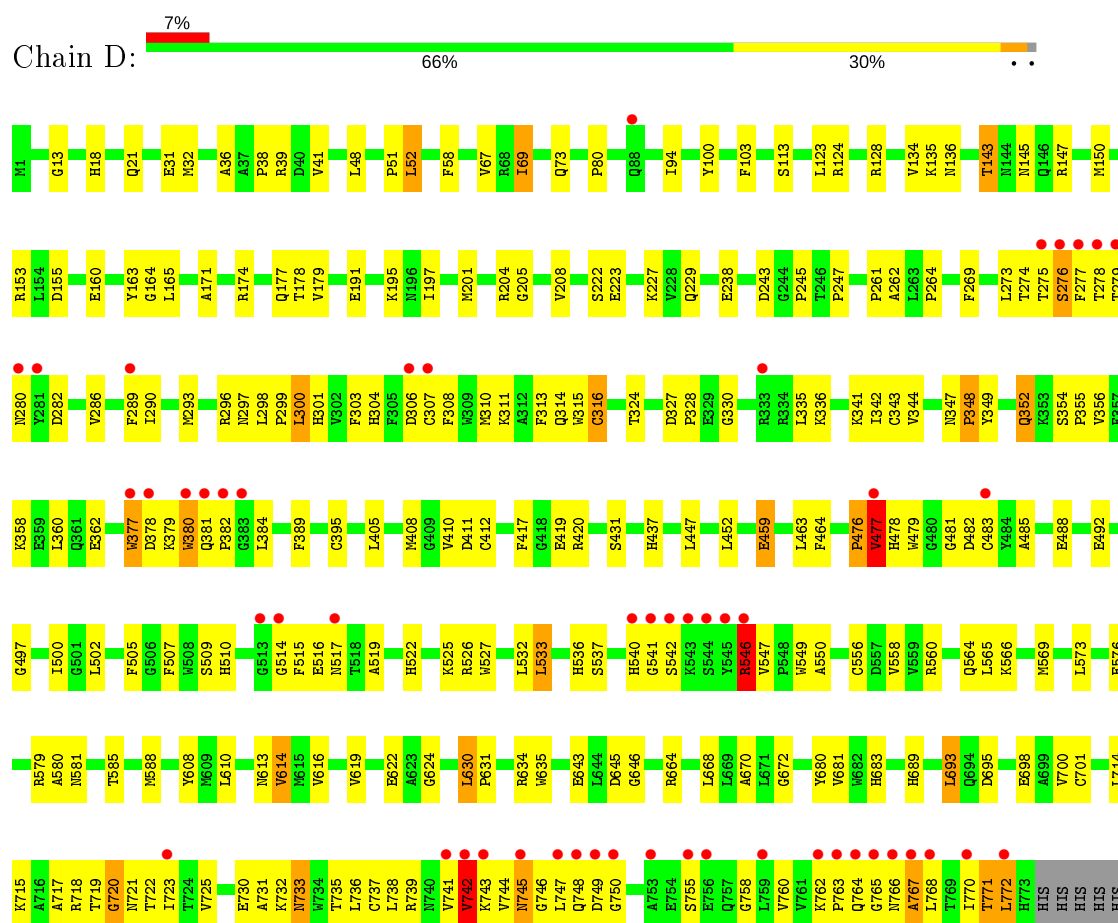
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	114	Total 114	O 114	0	0
5	C	167	Total 167	O 167	0	0
5	D	145	Total 145	O 145	0	0
5	E	122	Total 122	O 122	0	0
5	F	131	Total 131	O 131	0	0



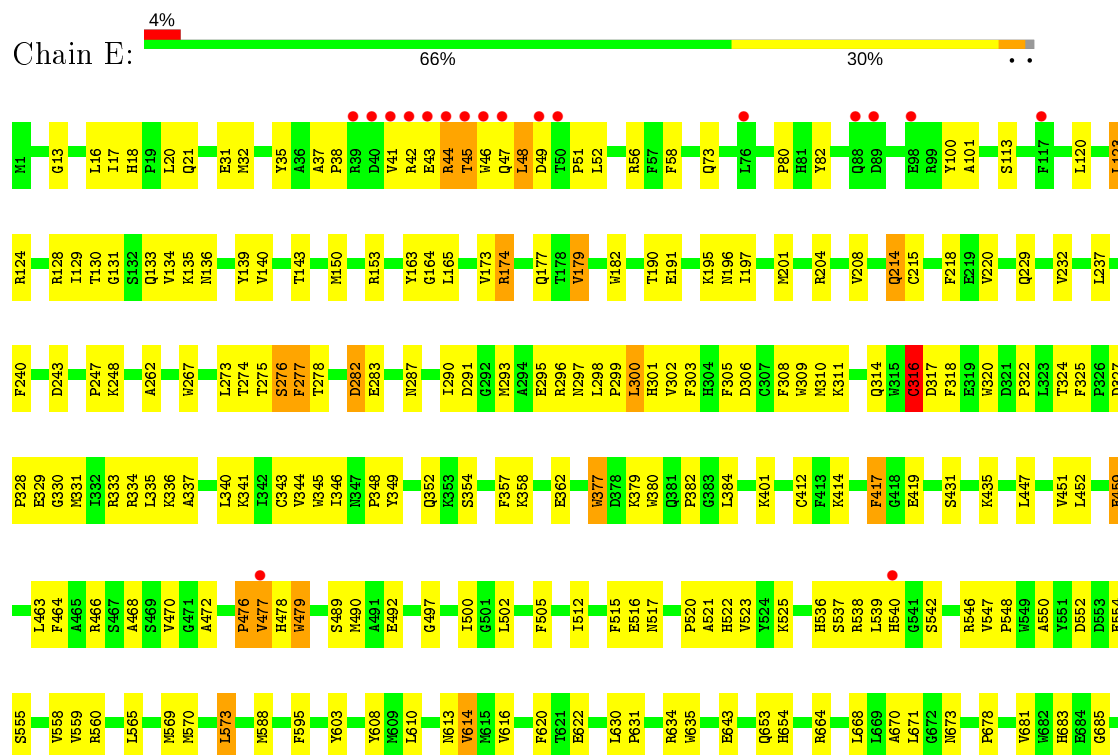
- Molecule 1: Putative family 31 glucosidase yicI

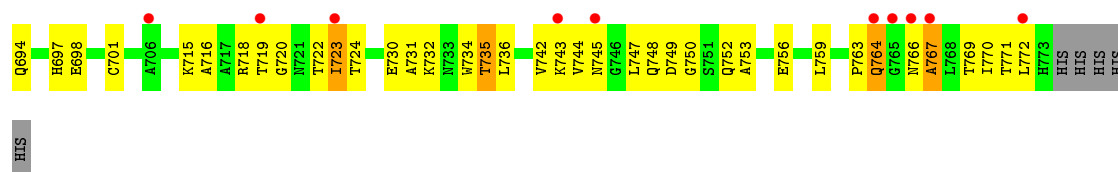


- Molecule 1: Putative family 31 glucosidase yicI

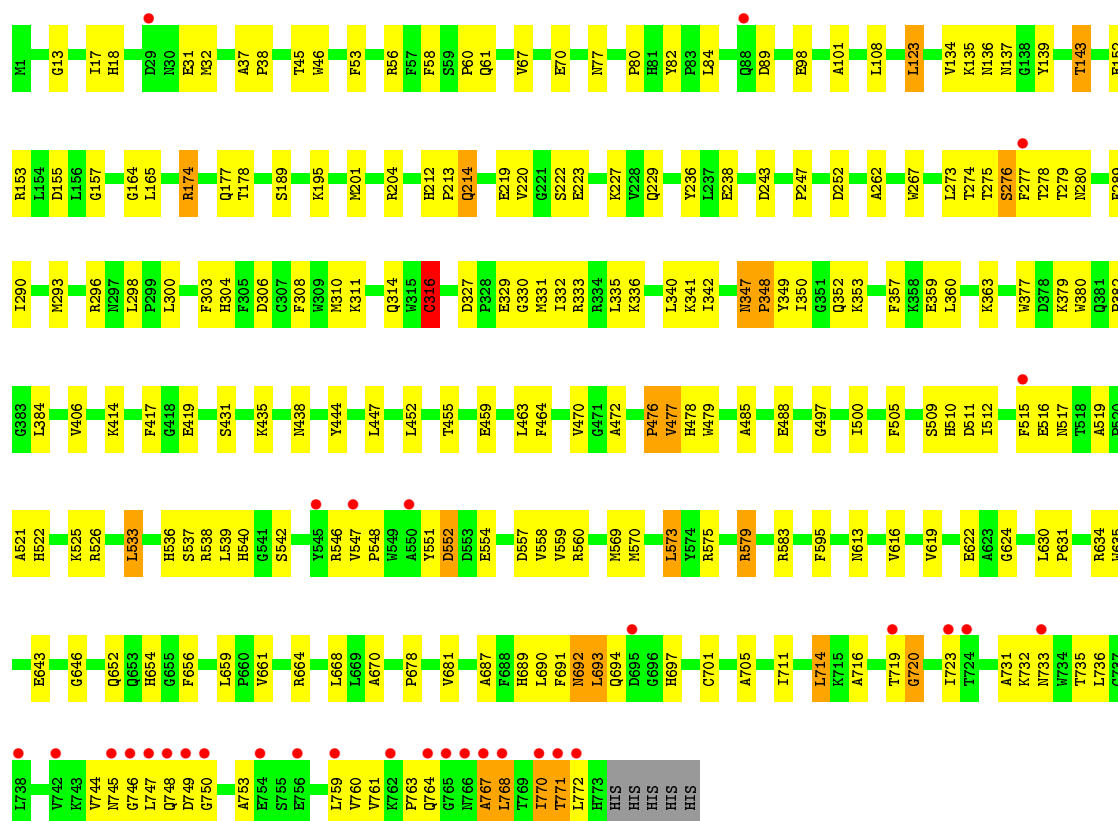


• Molecule 1: Putative family 31 glucosidase yicI





- Molecule 1: Putative family 31 glucosidase yicI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	162.14Å 175.47Å 210.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.20 69.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.88-2.20) 97.6 (69.48-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.272 0.227 , 0.224	Depositor DCC
R_{free} test set	15006 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	38360	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPO, SO4, XYF

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	0.41	0/6409	0.67	4/8711 (0.0%)
1	B	0.36	0/6409	0.62	1/8711 (0.0%)
1	C	0.41	0/6409	0.67	2/8711 (0.0%)
1	D	0.40	0/6409	0.65	1/8711 (0.0%)
1	E	0.40	0/6409	0.64	1/8711 (0.0%)
1	F	0.40	0/6409	0.65	2/8711 (0.0%)
All	All	0.40	0/38454	0.65	11/52266 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	316	CYS	CA-CB-SG	-6.24	102.77	114.00
1	C	316	CYS	CA-CB-SG	-6.16	102.92	114.00
1	E	613	ASN	N-CA-C	5.82	126.70	111.00
1	A	613	ASN	N-CA-C	5.81	126.67	111.00
1	D	613	ASN	N-CA-C	5.66	126.28	111.00
1	C	613	ASN	N-CA-C	5.56	126.01	111.00
1	F	613	ASN	N-CA-C	5.37	125.51	111.00
1	A	316	CYS	CA-CB-SG	-5.33	104.41	114.00
1	B	613	ASN	N-CA-C	5.12	124.84	111.00
1	A	464	PHE	N-CA-C	-5.06	97.34	111.00
1	A	476	PRO	N-CA-C	5.01	125.12	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6226	0	5934	195	0
1	B	6226	0	5934	199	0
1	C	6226	0	5934	213	0
1	D	6226	0	5934	214	0
1	E	6226	0	5934	224	0
1	F	6226	0	5934	191	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	25	0	0	2	0
3	A	10	0	6	2	0
3	B	10	0	6	1	0
3	C	10	0	6	2	0
3	E	10	0	6	2	0
4	B	13	0	15	0	0
4	C	13	0	15	0	0
4	D	13	0	15	0	0
4	E	13	0	15	0	0
5	A	168	0	0	3	0
5	B	114	0	0	6	0
5	C	167	0	0	5	0
5	D	145	0	0	5	0
5	E	122	0	0	4	0
5	F	131	0	0	6	0
All	All	38360	0	35688	1212	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 17.

All (1212) 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:A:274:THR:HG22	1:A:276:SER:H	1.14	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:THR:HG22	1:E:276:SER:H	1.00	1.09
1:A:668:LEU:HD21	1:A:714:LEU:HD12	1.39	1.04
1:C:579:ARG:HB2	1:C:579:ARG:HH11	1.21	1.04
1:C:32:MET:HE2	1:C:94:ILE:HG23	1.39	1.04
1:D:485:ALA:HB1	1:D:519:ALA:HB2	1.40	1.03
1:C:93:THR:HG22	1:C:104:LYS:HB3	1.40	1.02
1:B:719:THR:HG23	1:B:720:GLY:H	1.23	1.02
1:D:668:LEU:HD21	1:D:714:LEU:HD12	1.39	1.01
1:B:157:GLY:HA3	1:B:204:ARG:HH22	1.25	1.01
1:B:668:LEU:HD21	1:B:714:LEU:HD12	1.40	1.01
1:E:694:GLN:HB2	1:E:697:HIS:HD2	1.27	0.99
1:F:485:ALA:HB1	1:F:519:ALA:HB2	1.41	0.98
1:B:274:THR:HG22	1:B:276:SER:H	1.23	0.97
1:F:463:LEU:O	1:F:477:VAL:HG13	1.65	0.96
1:C:668:LEU:HD21	1:C:714:LEU:HD12	1.46	0.96
1:C:485:ALA:HB1	1:C:519:ALA:HB2	1.46	0.95
1:F:298:LEU:HD23	1:F:560:ARG:HG3	1.48	0.94
1:E:274:THR:HG21	1:E:540:HIS:ND1	1.81	0.94
1:F:274:THR:HG22	1:F:276:SER:H	1.29	0.94
1:A:485:ALA:HB1	1:A:519:ALA:HB2	1.50	0.94
1:E:463:LEU:O	1:E:477:VAL:HG13	1.68	0.93
1:D:381:GLN:HB2	1:D:384:LEU:HD12	1.52	0.91
1:E:274:THR:HG22	1:E:276:SER:N	1.84	0.91
1:B:694:GLN:HB2	1:B:697:HIS:HD2	1.36	0.90
1:C:274:THR:HG21	1:C:540:HIS:ND1	1.86	0.90
1:D:313:PHE:HA	1:D:381:GLN:HE22	1.38	0.89
1:F:668:LEU:HD21	1:F:714:LEU:HD13	1.53	0.88
1:D:547:VAL:HG23	1:D:550:ALA:HB2	1.55	0.87
1:D:280:ASN:HA	1:E:44:ARG:HH21	1.37	0.87
1:E:45:THR:HG23	1:E:46:TRP:HD1	1.39	0.87
1:C:579:ARG:CB	1:C:579:ARG:HH11	1.88	0.87
1:B:463:LEU:O	1:B:477:VAL:HG13	1.74	0.87
1:E:165:LEU:HD13	1:E:179:VAL:HG11	1.57	0.86
1:A:367:LEU:HG	1:A:425:VAL:HG21	1.59	0.85
1:D:273:LEU:HB2	1:D:300:LEU:HD21	1.59	0.84
1:C:425:VAL:HG22	1:C:426:GLN:N	1.91	0.83
1:C:368:LYS:O	1:C:425:VAL:HG23	1.79	0.83
1:F:694:GLN:HB2	1:F:697:HIS:HD2	1.42	0.83
1:E:214:GLN:HG3	1:E:435:LYS:HG2	1.61	0.82
1:F:634:ARG:HH21	1:F:643:GLU:HB3	1.45	0.82
1:D:766:ASN:C	1:D:768:LEU:H	1.82	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:O	1:A:425:VAL:HG23	1.79	0.82
1:A:463:LEU:O	1:A:477:VAL:HG22	1.81	0.81
1:C:329:GLU:HG3	1:C:408:MET:HG3	1.62	0.81
1:C:525:LYS:HG3	1:C:558:VAL:HG21	1.62	0.81
1:C:32:MET:CE	1:C:94:ILE:HG23	2.12	0.80
1:A:525:LYS:HG3	1:A:558:VAL:HG21	1.64	0.79
1:E:179:VAL:HG13	1:E:218:PHE:HB2	1.64	0.79
1:E:382:PRO:HG2	5:E:3048:HOH:O	1.82	0.79
1:B:136:ASN:HD21	1:B:227:LYS:HE3	1.47	0.79
1:F:274:THR:HG21	1:F:540:HIS:ND1	1.97	0.79
1:B:747:LEU:HD23	1:B:748:GLN:N	1.98	0.78
1:A:107:ASN:HD22	1:A:125:ASN:HD21	1.31	0.78
1:B:44:ARG:HA	1:B:47:GLN:HG3	1.65	0.78
1:E:525:LYS:HG2	1:E:558:VAL:HG21	1.64	0.78
1:A:723:ILE:HG12	1:A:770:ILE:HG13	1.65	0.77
1:A:195:LYS:HE2	1:A:478:HIS:HB3	1.66	0.77
1:F:13:GLY:O	1:F:143:THR:HB	1.85	0.77
1:B:719:THR:HG23	1:B:720:GLY:N	1.98	0.76
1:D:280:ASN:HA	1:E:44:ARG:NH2	2.00	0.76
1:C:201:MET:HE1	1:C:247:PRO:HB3	1.66	0.76
1:D:725:VAL:HB	1:D:768:LEU:HD12	1.67	0.76
1:A:274:THR:HG22	1:A:276:SER:N	1.95	0.76
1:C:762:LYS:HD2	1:C:763:PRO:HD2	1.68	0.76
1:D:541:GLY:HA3	1:D:546:ARG:HH21	1.50	0.75
1:E:723:ILE:HG13	1:E:770:ILE:HB	1.68	0.75
1:E:476:PRO:O	1:E:477:VAL:HG12	1.86	0.75
1:E:44:ARG:HG2	1:E:47:GLN:NE2	2.01	0.75
1:E:565:LEU:HG	1:E:569:MET:CE	2.17	0.75
1:A:761:VAL:HG11	1:A:768:LEU:HD21	1.69	0.75
1:D:540:HIS:C	1:D:546:ARG:HE	1.90	0.75
1:F:273:LEU:HB2	1:F:300:LEU:HD21	1.69	0.75
1:F:300:LEU:HD12	1:F:340:LEU:HD21	1.68	0.75
1:A:522:HIS:CE1	1:A:622:GLU:HG3	2.22	0.74
1:E:673:ASN:HD22	1:E:685:GLY:HA3	1.52	0.74
1:F:347:ASN:HD22	1:F:347:ASN:C	1.91	0.74
1:B:157:GLY:HA3	1:B:204:ARG:NH2	2.01	0.74
1:A:635:TRP:CH2	1:A:664:ARG:HG2	2.23	0.74
1:B:332:ILE:HD12	1:B:333:ARG:N	2.01	0.74
1:C:579:ARG:NH1	1:C:579:ARG:HB2	2.00	0.74
1:D:13:GLY:O	1:D:143:THR:HB	1.87	0.73
1:E:174:ARG:O	1:E:177:GLN:HG2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:694:GLN:HB2	1:E:697:HIS:CD2	2.19	0.73
1:B:689:HIS:ND1	1:B:739:ARG:NH1	2.36	0.73
1:C:274:THR:CG2	1:C:540:HIS:HA	2.18	0.73
1:B:32:MET:HE2	1:B:94:ILE:HG23	1.70	0.73
1:A:174:ARG:O	1:A:177:GLN:HG2	1.89	0.73
1:C:352:GLN:NE2	1:D:73:GLN:HG3	2.04	0.73
1:C:755:SER:HB3	1:C:758:GLY:O	1.88	0.73
1:A:750:GLY:HA2	1:A:764:GLN:HG2	1.71	0.72
1:A:762:LYS:HD2	1:A:763:PRO:HD2	1.72	0.72
1:A:367:LEU:CG	1:A:425:VAL:HG21	2.19	0.71
1:C:731:ALA:O	1:C:732:LYS:HD2	1.90	0.71
1:E:275:THR:O	1:E:276:SER:HB2	1.90	0.71
1:E:274:THR:CG2	1:E:276:SER:H	1.92	0.71
1:B:694:GLN:HB2	1:B:697:HIS:CD2	2.23	0.71
1:B:275:THR:O	1:B:276:SER:HB2	1.89	0.71
1:D:755:SER:HB3	1:D:758:GLY:O	1.90	0.71
1:C:174:ARG:O	1:C:177:GLN:HG2	1.90	0.71
1:D:377:TRP:HH2	1:D:420:ARG:HD3	1.54	0.71
1:B:274:THR:HG21	1:B:540:HIS:ND1	2.05	0.71
1:D:730:GLU:HG3	1:D:732:LYS:NZ	2.05	0.71
1:C:425:VAL:CG2	1:C:426:GLN:N	2.54	0.70
1:F:731:ALA:C	1:F:732:LYS:HD2	2.11	0.70
1:B:343:CYS:HB2	1:B:412:CYS:SG	2.31	0.70
1:F:694:GLN:HB2	1:F:697:HIS:CD2	2.25	0.70
1:D:522:HIS:CG	1:D:622:GLU:HG3	2.27	0.70
1:F:635:TRP:CH2	1:F:664:ARG:HG2	2.27	0.70
1:D:762:LYS:HD2	1:D:763:PRO:HD2	1.74	0.69
1:A:107:ASN:HD22	1:A:125:ASN:ND2	1.90	0.69
1:A:684:GLU:HG2	1:A:732:LYS:HB2	1.74	0.69
1:A:755:SER:HB3	1:A:758:GLY:O	1.91	0.69
1:D:485:ALA:HB1	1:D:519:ALA:CB	2.20	0.69
1:F:512:ILE:HB	1:F:539:LEU:HD23	1.74	0.69
1:D:32:MET:CE	1:D:94:ILE:HG23	2.23	0.69
1:C:725:VAL:HB	1:C:768:LEU:HB3	1.75	0.69
1:A:742:VAL:HG23	1:A:743:LYS:H	1.57	0.69
1:C:367:LEU:HD11	1:C:425:VAL:HG21	1.74	0.69
1:F:382:PRO:HG2	5:F:3046:HOH:O	1.91	0.69
1:B:522:HIS:CG	1:B:622:GLU:HG3	2.27	0.69
1:E:287:ASN:HD21	1:E:334:ARG:NH2	1.90	0.69
1:B:136:ASN:ND2	1:B:227:LYS:HE3	2.08	0.69
1:B:693:LEU:HD11	1:B:716:ALA:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:GLN:NE2	1:B:73:GLN:HG3	2.07	0.68
1:B:742:VAL:HG23	1:B:743:LYS:H	1.58	0.68
1:F:311:LYS:HE3	1:F:314:GLN:OE1	1.93	0.68
1:E:165:LEU:CD1	1:E:179:VAL:HG11	2.23	0.68
1:A:548:PRO:HG3	1:A:559:VAL:HG21	1.76	0.67
1:C:367:LEU:CD1	1:C:425:VAL:HG21	2.24	0.67
1:A:165:LEU:HD13	1:A:179:VAL:HG11	1.75	0.67
1:C:731:ALA:C	1:C:732:LYS:HD2	2.15	0.67
1:D:742:VAL:HG23	1:D:743:LYS:H	1.59	0.67
1:E:673:ASN:ND2	1:E:685:GLY:HA3	2.08	0.67
1:C:133:GLN:HB2	1:C:136:ASN:HD22	1.59	0.67
1:F:347:ASN:ND2	1:F:349:TYR:H	1.93	0.67
1:D:36:ALA:O	1:D:52:LEU:HD23	1.95	0.67
1:D:541:GLY:HA3	1:D:546:ARG:NH2	2.09	0.67
1:A:274:THR:HG21	1:A:540:HIS:ND1	2.09	0.66
1:E:13:GLY:O	1:E:143:THR:HB	1.95	0.66
1:B:174:ARG:O	1:B:177:GLN:HG2	1.95	0.66
1:C:274:THR:HG22	1:C:540:HIS:HA	1.77	0.66
1:D:731:ALA:C	1:D:732:LYS:HD2	2.16	0.66
1:B:195:LYS:HE2	1:B:478:HIS:HB3	1.78	0.66
1:C:532:LEU:O	1:C:566:LYS:HD2	1.94	0.66
1:D:343:CYS:HB2	1:D:412:CYS:SG	2.36	0.66
1:D:730:GLU:HG3	1:D:732:LYS:HZ2	1.61	0.66
1:F:763:PRO:HB3	1:F:768:LEU:HD22	1.78	0.66
1:D:262:ALA:HB3	1:D:476:PRO:HG3	1.79	0.65
1:A:165:LEU:HD12	1:A:174:ARG:HG2	1.78	0.65
1:C:512:ILE:HB	1:C:539:LEU:HD23	1.77	0.65
1:A:347:ASN:HD22	1:A:347:ASN:C	1.99	0.65
1:B:719:THR:CG2	1:B:720:GLY:H	2.05	0.65
1:F:705:ALA:HB2	1:F:711:ILE:HB	1.78	0.65
1:D:380:TRP:HA	1:E:49:ASP:OD1	1.97	0.65
1:D:747:LEU:HD23	1:D:748:GLN:N	2.12	0.65
1:F:174:ARG:O	1:F:177:GLN:HG2	1.96	0.65
1:A:500:ILE:HG12	1:A:505:PHE:HB2	1.78	0.65
1:D:136:ASN:HB3	1:D:153:ARG:HB2	1.79	0.65
1:D:276:SER:HB2	1:D:279:THR:HG23	1.78	0.65
1:E:377:TRP:CZ3	1:E:379:LYS:HD2	2.31	0.65
1:A:16:LEU:HD22	1:A:140:VAL:HG22	1.79	0.65
1:B:123:LEU:N	1:B:123:LEU:HD22	2.11	0.65
1:C:692:ASN:HD22	1:C:692:ASN:H	1.43	0.65
1:D:485:ALA:CB	1:D:519:ALA:HB2	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:GLU:O	1:E:333:ARG:HG2	1.97	0.65
1:C:638:LEU:O	1:C:739:ARG:NH2	2.30	0.65
1:D:540:HIS:CG	1:D:541:GLY:H	2.14	0.65
1:E:417:PHE:HA	1:E:419:GLU:OE2	1.97	0.64
1:C:165:LEU:HD12	1:C:174:ARG:HG2	1.79	0.64
1:F:417:PHE:HA	1:F:419:GLU:OE2	1.97	0.64
1:C:730:GLU:HG3	1:C:732:LYS:NZ	2.13	0.64
1:A:201:MET:HE1	1:A:247:PRO:HA	1.78	0.64
1:C:300:LEU:HD13	1:C:301:HIS:N	2.13	0.64
1:C:367:LEU:CG	1:C:425:VAL:HG21	2.27	0.64
1:D:417:PHE:HA	1:D:419:GLU:OE2	1.97	0.64
1:E:476:PRO:O	1:E:477:VAL:CG1	2.45	0.64
1:E:565:LEU:HG	1:E:569:MET:HE2	1.78	0.64
1:B:32:MET:CE	1:B:94:ILE:HG23	2.27	0.64
1:D:32:MET:HE2	1:D:94:ILE:HG23	1.79	0.64
1:F:692:ASN:H	1:F:692:ASN:HD22	1.46	0.64
1:A:274:THR:HG22	1:A:275:THR:N	2.13	0.64
1:B:329:GLU:O	1:B:332:ILE:HG13	1.98	0.64
1:B:681:VAL:O	1:B:681:VAL:HG13	1.97	0.64
1:D:565:LEU:HG	1:D:569:MET:HE2	1.80	0.64
1:B:485:ALA:HB1	1:B:519:ALA:HB2	1.78	0.64
1:B:748:GLN:HB2	1:B:769:THR:H	1.62	0.63
1:A:382:PRO:HG2	5:A:3018:HOH:O	1.97	0.63
1:C:31:GLU:OE1	1:C:56:ARG:HD3	1.99	0.63
1:C:692:ASN:N	1:C:692:ASN:HD22	1.96	0.63
1:F:274:THR:HG23	1:F:304:HIS:HD2	1.63	0.63
1:C:153:ARG:HG2	1:C:229:GLN:HB2	1.80	0.63
1:C:367:LEU:HG	1:C:425:VAL:HG21	1.81	0.63
1:C:698:GLU:HG3	1:C:717:ALA:HB2	1.81	0.63
1:D:746:GLY:H	1:D:771:THR:HG23	1.63	0.63
1:B:459:GLU:CD	1:B:459:GLU:H	2.00	0.63
1:B:476:PRO:O	1:B:477:VAL:HG12	1.99	0.63
1:F:476:PRO:O	1:F:477:VAL:HG12	1.99	0.63
1:C:768:LEU:HD13	1:C:769:THR:N	2.14	0.63
1:F:31:GLU:HG2	1:F:58:PHE:HB3	1.82	0.62
1:A:747:LEU:HD22	1:A:750:GLY:O	1.98	0.62
1:B:752:GLN:HB2	1:B:759:LEU:HD11	1.80	0.62
1:A:212:HIS:CE1	1:A:238:GLU:H	2.18	0.62
1:C:82:TYR:HB2	1:C:84:LEU:HD21	1.81	0.62
1:E:16:LEU:HD22	1:E:140:VAL:HG22	1.80	0.62
1:D:565:LEU:HG	1:D:569:MET:CE	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:ALA:HB3	1:E:476:PRO:HG3	1.81	0.62
1:F:634:ARG:NH2	1:F:643:GLU:HB3	2.14	0.62
1:B:347:ASN:C	1:B:347:ASN:HD22	2.03	0.62
1:D:532:LEU:O	1:D:566:LYS:HD2	2.00	0.62
1:A:341:LYS:C	1:A:342:ILE:HD12	2.20	0.62
1:B:521:ALA:HB3	5:B:3120:HOH:O	1.99	0.62
1:D:540:HIS:CG	1:D:541:GLY:N	2.67	0.62
1:F:681:VAL:HG13	1:F:681:VAL:O	2.00	0.62
1:B:274:THR:HG22	1:B:275:THR:N	2.15	0.61
1:C:382:PRO:HG2	5:C:3013:HOH:O	2.00	0.61
1:C:693:LEU:HD11	1:C:716:ALA:O	2.00	0.61
1:D:546:ARG:HA	1:D:546:ARG:HH11	1.66	0.61
1:E:320:TRP:O	1:E:322:PRO:HD3	1.99	0.61
1:A:273:LEU:HD13	1:A:274:THR:N	2.15	0.61
1:C:425:VAL:CG2	1:C:426:GLN:H	2.13	0.61
1:C:579:ARG:CG	1:C:579:ARG:HH11	2.13	0.61
1:E:753:ALA:O	1:E:759:LEU:HD12	2.00	0.61
1:E:18:HIS:O	1:E:38:PRO:HA	2.00	0.61
1:B:307:CYS:HB3	1:B:315:TRP:CZ2	2.36	0.61
1:C:275:THR:O	1:C:276:SER:HB2	2.01	0.61
1:D:744:VAL:HG21	1:D:770:ILE:HG23	1.83	0.61
1:A:425:VAL:HG22	1:A:426:GLN:N	2.14	0.61
1:B:766:ASN:O	1:B:767:ALA:HB3	2.00	0.61
1:F:195:LYS:HE2	1:F:478:HIS:HB3	1.83	0.61
1:C:689:HIS:ND1	1:C:739:ARG:NH1	2.48	0.61
1:D:379:LYS:O	1:D:380:TRP:HB3	2.01	0.61
1:D:195:LYS:HE2	1:D:478:HIS:HB3	1.81	0.61
1:E:100:TYR:HD2	1:E:113:SER:HA	1.66	0.61
1:C:300:LEU:HD12	1:C:340:LEU:CD2	2.30	0.61
1:F:275:THR:O	1:F:276:SER:HB2	2.01	0.61
1:B:212:HIS:HE1	1:B:238:GLU:H	1.49	0.60
1:C:347:ASN:HD22	1:C:347:ASN:C	2.04	0.60
1:F:631:PRO:HD2	1:F:635:TRP:CZ2	2.35	0.60
1:B:690:LEU:HD21	1:B:693:LEU:HD12	1.83	0.60
1:C:522:HIS:CG	1:C:622:GLU:HG3	2.37	0.60
1:A:414:LYS:HZ2	1:A:538:ARG:HH12	1.49	0.60
1:A:2:LYS:HE3	1:D:191:GLU:OE2	2.01	0.60
1:D:766:ASN:C	1:D:768:LEU:N	2.53	0.60
1:E:273:LEU:HB2	1:E:300:LEU:HD21	1.82	0.60
1:E:21:GLN:NE2	1:E:42:ARG:HG3	2.17	0.60
1:F:579:ARG:HG3	1:F:579:ARG:HH11	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:PHE:HA	1:C:419:GLU:OE2	2.02	0.60
1:B:742:VAL:HG23	1:B:743:LYS:N	2.15	0.60
1:C:547:VAL:HG23	1:C:550:ALA:HB2	1.83	0.60
1:E:565:LEU:HG	1:E:569:MET:HE1	1.84	0.60
1:E:772:LEU:HD22	1:E:772:LEU:H	1.65	0.60
1:F:540:HIS:C	1:F:546:ARG:HG3	2.22	0.60
1:F:296:ARG:O	1:F:560:ARG:NH1	2.35	0.60
1:A:290:ILE:CD1	1:A:335:LEU:HD22	2.32	0.60
1:A:368:LYS:O	1:A:425:VAL:CG2	2.50	0.59
1:B:547:VAL:HG23	1:B:550:ALA:HB2	1.82	0.59
1:D:731:ALA:O	1:D:732:LYS:HD2	2.02	0.59
1:E:274:THR:HG21	1:E:540:HIS:CE1	2.36	0.59
1:D:463:LEU:O	1:D:477:VAL:HG13	2.01	0.59
1:F:347:ASN:C	1:F:347:ASN:ND2	2.55	0.59
1:B:311:LYS:HE3	1:B:314:GLN:OE1	2.02	0.59
1:F:750:GLY:HA2	1:F:764:GLN:HG2	1.84	0.59
1:C:300:LEU:HD12	1:C:340:LEU:HD22	1.83	0.59
1:C:463:LEU:O	1:C:477:VAL:HB	2.02	0.59
1:C:684:GLU:HG2	1:C:732:LYS:HB2	1.85	0.59
1:D:546:ARG:CA	1:D:546:ARG:HH11	2.15	0.59
1:E:31:GLU:OE1	1:E:56:ARG:HD3	2.02	0.59
1:F:681:VAL:HG12	2:F:3005:SO4:O3	2.02	0.59
1:A:163:TYR:HB3	1:A:502:LEU:HD13	1.85	0.59
1:B:671:LEU:HD12	1:B:671:LEU:N	2.18	0.59
1:A:342:ILE:HD12	1:A:342:ILE:N	2.18	0.59
1:B:123:LEU:HA	1:B:127:GLU:O	2.03	0.59
1:F:352:GLN:HA	1:F:357:PHE:CD2	2.37	0.59
1:B:31:GLU:OE1	1:B:56:ARG:HD3	2.02	0.59
1:B:748:GLN:CG	1:B:769:THR:HB	2.32	0.59
1:D:476:PRO:O	1:D:477:VAL:HG13	2.03	0.58
1:A:212:HIS:HE1	1:A:238:GLU:H	1.49	0.58
1:C:343:CYS:HB2	1:C:412:CYS:SG	2.42	0.58
1:D:124:ARG:NH2	1:D:243:ASP:OD1	2.34	0.58
1:E:635:TRP:CH2	1:E:664:ARG:HG2	2.38	0.58
1:B:695:ASP:HA	1:B:718:ARG:HD3	1.85	0.58
1:E:515:PHE:HD1	1:E:516:GLU:HG2	1.68	0.58
1:E:123:LEU:HD22	1:E:123:LEU:N	2.18	0.58
1:C:273:LEU:HD13	1:C:274:THR:N	2.19	0.58
1:C:274:THR:HG21	1:C:540:HIS:HA	1.85	0.58
1:E:520:PRO:O	1:E:521:ALA:HB3	2.03	0.58
1:F:123:LEU:HD22	1:F:123:LEU:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:GLU:HG2	1:C:58:PHE:HB3	1.85	0.58
1:C:631:PRO:O	1:C:646:GLY:HA3	2.03	0.58
1:D:352:GLN:OE1	1:E:73:GLN:N	2.33	0.58
1:D:747:LEU:HD22	1:D:750:GLY:O	2.04	0.58
1:E:536:HIS:HA	5:E:3025:HOH:O	2.04	0.58
1:F:300:LEU:HD12	1:F:340:LEU:CD2	2.34	0.58
1:F:310:MET:SD	1:F:316:CYS:HA	2.44	0.58
1:E:214:GLN:HE22	1:E:232:VAL:CG2	2.17	0.58
1:E:516:GLU:O	1:E:517:ASN:HB2	2.03	0.58
1:F:747:LEU:HD22	1:F:750:GLY:O	2.04	0.58
1:A:134:VAL:O	1:A:135:LYS:HB2	2.04	0.57
1:A:347:ASN:ND2	1:A:347:ASN:C	2.58	0.57
1:A:516:GLU:O	1:A:517:ASN:HB2	2.04	0.57
1:B:348:PRO:O	1:B:387:TYR:HD1	1.87	0.57
1:B:714:LEU:HD13	1:B:715:LYS:N	2.20	0.57
1:F:595:PHE:CE1	1:F:631:PRO:HG2	2.39	0.57
1:B:719:THR:HG22	1:B:722:THR:O	2.03	0.57
1:A:736:LEU:HD13	1:A:736:LEU:C	2.25	0.57
1:D:525:LYS:HG2	1:D:558:VAL:HG21	1.86	0.57
1:F:733:ASN:OD1	1:F:733:ASN:O	2.21	0.57
1:D:695:ASP:HA	1:D:718:ARG:HD3	1.86	0.57
1:E:547:VAL:HG23	1:E:550:ALA:HB2	1.86	0.57
1:F:447:LEU:C	1:F:447:LEU:HD23	2.24	0.57
1:F:719:THR:HG23	1:F:720:GLY:N	2.20	0.57
1:F:548:PRO:HG3	1:F:559:VAL:HG21	1.86	0.57
1:A:580:ALA:HA	1:A:585:THR:O	2.04	0.57
1:B:28:GLN:NE2	1:B:33:VAL:HG21	2.19	0.57
1:C:123:LEU:HD22	1:C:123:LEU:N	2.20	0.57
1:C:165:LEU:HD13	1:C:179:VAL:HG21	1.87	0.57
1:E:35:TYR:HB3	1:E:52:LEU:HD11	1.87	0.57
1:A:123:LEU:HD13	1:A:128:ARG:HA	1.85	0.57
1:D:298:LEU:CD2	1:D:560:ARG:HB2	2.35	0.57
1:B:512:ILE:HB	1:B:539:LEU:HD23	1.87	0.56
1:E:201:MET:HE1	1:E:247:PRO:HA	1.87	0.56
1:B:278:THR:HG21	1:F:45:THR:HA	1.86	0.56
1:A:742:VAL:HG23	1:A:743:LYS:N	2.21	0.56
1:D:631:PRO:O	1:D:646:GLY:HA3	2.05	0.56
1:E:204:ARG:HH11	1:E:204:ARG:HG2	1.69	0.56
1:F:204:ARG:HG2	1:F:204:ARG:O	2.05	0.56
1:A:153:ARG:HG2	1:A:229:GLN:HB2	1.87	0.56
1:A:377:TRP:CZ3	1:A:379:LYS:HD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:LEU:HD23	1:C:384:LEU:C	2.25	0.56
1:D:349:TYR:HB3	1:D:384:LEU:HD21	1.87	0.56
1:D:377:TRP:CZ3	1:D:379:LYS:HD2	2.40	0.56
1:E:522:HIS:CG	1:E:622:GLU:HG3	2.40	0.56
1:B:314:GLN:HB3	1:B:354:SER:HB2	1.86	0.56
1:D:174:ARG:O	1:D:177:GLN:HG2	2.04	0.56
1:C:195:LYS:HE2	1:C:478:HIS:HB3	1.87	0.56
1:C:93:THR:CG2	1:C:104:LYS:HB3	2.25	0.56
1:C:134:VAL:O	1:C:135:LYS:HB2	2.06	0.56
1:C:296:ARG:O	1:C:560:ARG:NH1	2.39	0.56
1:E:174:ARG:HB3	1:E:220:VAL:HG11	1.87	0.56
1:E:539:LEU:HB3	1:E:546:ARG:HB3	1.88	0.56
1:A:275:THR:O	1:A:276:SER:HB2	2.04	0.56
1:B:350:ILE:HD13	1:B:360:LEU:HD12	1.87	0.56
1:C:516:GLU:O	1:C:517:ASN:HB2	2.06	0.56
1:F:137:ASN:HB3	1:F:152:GLU:OE1	2.05	0.56
1:F:485:ALA:HB1	1:F:519:ALA:CB	2.25	0.56
1:E:311:LYS:HE3	1:E:314:GLN:OE1	2.06	0.56
1:B:476:PRO:O	1:B:477:VAL:CG1	2.53	0.56
1:C:290:ILE:CD1	1:C:335:LEU:HD22	2.36	0.56
1:F:348:PRO:HG2	1:F:349:TYR:CE1	2.40	0.56
1:B:347:ASN:ND2	1:B:347:ASN:C	2.59	0.56
1:F:155:ASP:OD1	1:F:227:LYS:HE3	2.06	0.56
1:A:212:HIS:HE1	1:A:237:LEU:HD12	1.70	0.55
1:A:48:LEU:HD12	1:A:49:ASP:HB2	1.88	0.55
1:B:164:GLY:O	1:B:165:LEU:HB2	2.06	0.55
1:A:692:ASN:HD22	1:A:692:ASN:H	1.52	0.55
1:C:18:HIS:O	1:C:38:PRO:HA	2.06	0.55
1:F:165:LEU:HD12	1:F:174:ARG:HG2	1.88	0.55
1:F:476:PRO:O	1:F:477:VAL:CG1	2.54	0.55
1:F:746:GLY:N	1:F:771:THR:HG23	2.21	0.55
1:C:124:ARG:NH2	1:C:243:ASP:OD1	2.38	0.55
1:C:525:LYS:CG	1:C:558:VAL:HG21	2.33	0.55
1:D:459:GLU:CD	1:D:459:GLU:H	2.06	0.55
1:B:695:ASP:OD1	1:B:720:GLY:HA2	2.07	0.55
1:D:18:HIS:O	1:D:38:PRO:HA	2.07	0.55
1:D:482:ASP:HB3	1:D:516:GLU:OE1	2.07	0.55
1:A:43:GLU:HB2	1:A:46:TRP:HD1	1.71	0.55
1:A:770:ILE:HD12	1:A:770:ILE:C	2.27	0.55
1:C:459:GLU:H	1:C:459:GLU:CD	2.02	0.55
1:E:44:ARG:HG2	1:E:47:GLN:HE22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:LYS:HD2	1:B:763:PRO:HD2	1.88	0.55
1:E:742:VAL:HG23	1:E:743:LYS:N	2.22	0.55
1:B:500:ILE:HG12	1:B:505:PHE:HB2	1.88	0.55
1:D:672:GLY:HA3	1:D:680:TYR:OH	2.07	0.55
1:D:735:THR:CG2	1:D:736:LEU:N	2.70	0.55
1:E:195:LYS:HE2	1:E:478:HIS:HB3	1.87	0.55
1:B:744:VAL:HG22	1:B:771:THR:O	2.06	0.55
1:D:631:PRO:HD2	1:D:635:TRP:CZ2	2.41	0.55
1:A:447:LEU:C	1:A:447:LEU:HD23	2.27	0.55
1:B:285:THR:O	1:B:288:SER:HB3	2.07	0.55
1:C:348:PRO:HG2	1:C:349:TYR:CE1	2.42	0.55
1:B:730:GLU:HG3	1:B:732:LYS:NZ	2.22	0.54
1:F:274:THR:HG21	1:F:540:HIS:CE1	2.42	0.54
1:B:648:ARG:HD3	5:C:3115:HOH:O	2.06	0.54
1:B:722:THR:HG23	1:B:769:THR:HG23	1.89	0.54
1:D:136:ASN:ND2	1:D:227:LYS:HE2	2.22	0.54
1:E:447:LEU:C	1:E:447:LEU:HD23	2.28	0.54
1:E:718:ARG:HB2	1:E:723:ILE:HG22	1.89	0.54
1:C:261:PRO:HA	1:C:473:GLN:O	2.08	0.54
1:C:347:ASN:ND2	1:C:347:ASN:C	2.61	0.54
1:E:133:GLN:HB2	1:E:136:ASN:HD22	1.72	0.54
1:E:500:ILE:HG12	1:E:505:PHE:HB2	1.89	0.54
1:E:479:TRP:CZ2	3:E:804:XYF:H4	2.42	0.54
1:F:744:VAL:HG22	1:F:745:ASN:N	2.22	0.54
1:B:382:PRO:HG2	5:B:3011:HOH:O	2.08	0.54
1:B:671:LEU:HD13	1:B:689:HIS:CD2	2.43	0.54
1:F:273:LEU:HD13	1:F:274:THR:N	2.22	0.54
1:F:331:MET:O	1:F:335:LEU:HG	2.08	0.54
1:A:571:PRO:HB2	1:A:670:ALA:O	2.06	0.54
1:D:700:VAL:HG22	1:D:715:LYS:HG2	1.90	0.54
1:E:744:VAL:HG22	1:E:745:ASN:N	2.23	0.54
1:F:350:ILE:HD13	1:F:360:LEU:HD12	1.88	0.54
1:B:13:GLY:O	1:B:143:THR:HB	2.07	0.54
1:E:681:VAL:HG23	1:E:683:HIS:CE1	2.43	0.54
1:F:526:ARG:HD2	1:F:619:VAL:HB	1.90	0.54
1:F:575:ARG:NH2	1:F:579:ARG:HH12	2.05	0.54
1:B:201:MET:CE	1:B:247:PRO:HB3	2.38	0.54
1:C:277:PHE:CD2	1:C:278:THR:HG23	2.42	0.54
1:C:575:ARG:NH1	1:C:579:ARG:HH12	2.05	0.54
1:D:735:THR:CG2	1:D:760:VAL:HG13	2.38	0.54
1:E:522:HIS:CE1	1:E:523:VAL:HG23	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:TRP:HZ2	3:B:802:XYF:H4	1.73	0.54
1:C:136:ASN:HB3	1:C:153:ARG:HB2	1.89	0.54
1:C:20:LEU:HD22	1:C:134:VAL:CG2	2.38	0.54
1:C:291:ASP:O	1:C:295:GLU:HG3	2.08	0.54
1:C:695:ASP:OD1	1:C:719:THR:O	2.25	0.54
1:E:128:ARG:HH22	1:E:131:GLY:HA3	1.72	0.54
1:F:336:LYS:HG2	1:F:342:ILE:CD1	2.37	0.54
1:A:479:TRP:HZ2	3:A:801:XYF:H4	1.73	0.54
1:E:352:GLN:HA	1:E:357:PHE:CD2	2.43	0.54
1:F:17:ILE:HG12	1:F:139:TYR:HB3	1.90	0.54
1:F:384:LEU:HD23	1:F:384:LEU:C	2.28	0.54
1:C:681:VAL:O	1:C:681:VAL:HG23	2.07	0.53
1:A:336:LYS:HG2	1:A:342:ILE:HD13	1.90	0.53
1:C:327:ASP:OD2	1:C:330:GLY:HA3	2.06	0.53
1:D:483:CYS:SG	1:D:514:GLY:HA2	2.48	0.53
1:A:766:ASN:O	1:A:767:ALA:HB2	2.08	0.53
1:D:772:LEU:H	1:D:772:LEU:HD22	1.72	0.53
1:F:735:THR:HG22	1:F:736:LEU:N	2.23	0.53
1:A:311:LYS:HE3	1:A:314:GLN:OE1	2.08	0.53
1:D:336:LYS:HE3	1:D:411:ASP:OD2	2.09	0.53
1:E:459:GLU:H	1:E:459:GLU:CD	2.12	0.53
1:E:735:THR:CG2	1:E:736:LEU:N	2.72	0.53
1:B:310:MET:SD	1:B:316:CYS:HA	2.49	0.53
1:F:267:TRP:CE3	1:F:341:LYS:HG3	2.44	0.53
1:F:497:GLY:O	1:F:500:ILE:HG22	2.09	0.53
1:F:668:LEU:O	1:F:701:CYS:HB2	2.09	0.53
1:A:136:ASN:HB3	1:A:153:ARG:HB2	1.90	0.53
1:C:447:LEU:C	1:C:447:LEU:HD23	2.28	0.53
1:E:745:ASN:HB3	1:E:771:THR:O	2.09	0.53
1:F:70:GLU:HB3	1:F:236:TYR:HB2	1.90	0.53
1:A:17:ILE:HG13	1:A:17:ILE:O	2.07	0.53
1:B:352:GLN:HA	1:B:357:PHE:CD2	2.43	0.53
1:B:315:TRP:HB2	1:B:381:GLN:OE1	2.09	0.53
1:B:668:LEU:HD13	1:B:690:LEU:HD13	1.91	0.53
1:C:694:GLN:HB2	1:C:697:HIS:CD2	2.44	0.53
1:D:282:ASP:O	1:D:286:VAL:HG23	2.09	0.53
1:D:310:MET:SD	1:D:316:CYS:HA	2.48	0.53
1:E:333:ARG:HH11	1:E:336:LYS:HE3	1.73	0.53
1:E:552:ASP:OD1	1:E:555:SER:N	2.38	0.53
1:F:472:ALA:HB1	5:F:3084:HOH:O	2.08	0.53
1:B:16:LEU:HD22	1:B:140:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:742:VAL:HG23	1:C:743:LYS:N	2.24	0.53
1:D:509:SER:HB3	1:D:536:HIS:HB2	1.91	0.53
1:D:547:VAL:CG2	1:D:550:ALA:HB2	2.34	0.53
1:E:749:ASP:C	1:E:764:GLN:HE22	2.13	0.53
1:F:153:ARG:HG2	1:F:229:GLN:HB2	1.91	0.53
1:F:277:PHE:CD2	1:F:278:THR:HG23	2.44	0.53
1:A:343:CYS:HB2	1:A:412:CYS:SG	2.49	0.52
1:E:681:VAL:HG13	1:E:681:VAL:O	2.09	0.52
1:F:274:THR:HG22	1:F:275:THR:N	2.25	0.52
1:B:262:ALA:HB3	1:B:476:PRO:HG3	1.90	0.52
1:B:61:GLN:NE2	1:B:87:LEU:HG	2.23	0.52
1:E:742:VAL:HG23	1:E:743:LYS:H	1.74	0.52
1:E:744:VAL:HG21	1:E:770:ILE:CG2	2.39	0.52
1:C:273:LEU:HB2	1:C:300:LEU:HD21	1.91	0.52
1:D:735:THR:HG22	1:D:736:LEU:N	2.24	0.52
1:B:298:LEU:CD2	1:B:560:ARG:HB2	2.39	0.52
1:C:453:LYS:HD2	1:C:458:GLU:OE1	2.09	0.52
1:D:155:ASP:OD1	1:D:227:LYS:HE3	2.09	0.52
1:E:595:PHE:CE1	1:E:631:PRO:HG2	2.43	0.52
1:C:515:PHE:HD1	1:C:516:GLU:HG2	1.74	0.52
1:D:736:LEU:C	1:D:736:LEU:HD13	2.29	0.52
1:D:766:ASN:O	1:D:768:LEU:N	2.42	0.52
1:E:267:TRP:CE3	1:E:341:LYS:HG3	2.44	0.52
1:F:174:ARG:HB3	1:F:220:VAL:HG11	1.92	0.52
1:F:327:ASP:OD2	1:F:330:GLY:HA3	2.08	0.52
1:F:719:THR:HG23	1:F:720:GLY:H	1.73	0.52
1:A:588:MET:HE3	5:A:3065:HOH:O	2.08	0.52
1:B:479:TRP:HA	1:B:509:SER:O	2.10	0.52
1:C:201:MET:CE	1:C:247:PRO:HB3	2.38	0.52
1:E:43:GLU:C	1:E:45:THR:H	2.13	0.52
1:E:468:ALA:HB1	1:E:472:ALA:HB3	1.91	0.52
1:A:212:HIS:CE1	1:A:237:LEU:HD12	2.45	0.52
1:A:43:GLU:HB3	1:A:45:THR:HG22	1.90	0.52
1:E:290:ILE:CD1	1:E:335:LEU:HD22	2.39	0.52
1:A:719:THR:HG23	1:A:720:GLY:H	1.75	0.52
1:A:80:PRO:HD3	1:A:431:SER:HB3	1.91	0.52
1:B:384:LEU:HD23	1:B:384:LEU:C	2.31	0.52
1:F:557:ASP:OD1	1:F:560:ARG:NH2	2.43	0.52
1:D:719:THR:HG22	1:D:722:THR:HB	1.92	0.52
1:E:479:TRP:CH2	3:E:804:XYF:H4	2.45	0.52
1:F:290:ILE:CD1	1:F:335:LEU:HD22	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:PRO:HD3	1:D:431:SER:HB3	1.91	0.52
1:D:681:VAL:HG13	1:D:681:VAL:O	2.09	0.52
1:E:476:PRO:C	1:E:477:VAL:HG12	2.29	0.52
1:E:744:VAL:HG22	1:E:771:THR:O	2.10	0.52
1:F:516:GLU:O	1:F:517:ASN:HB2	2.09	0.52
1:A:466:ARG:HB2	1:A:479:TRP:CH2	2.44	0.51
1:D:134:VAL:O	1:D:135:LYS:HB2	2.10	0.51
1:D:274:THR:O	1:D:546:ARG:HG3	2.10	0.51
1:D:721:ASN:O	1:D:771:THR:HA	2.10	0.51
1:A:347:ASN:HA	1:A:444:TYR:OH	2.11	0.51
1:C:18:HIS:HB2	1:C:20:LEU:HD21	1.91	0.51
1:D:31:GLU:HG2	1:D:58:PHE:HB3	1.92	0.51
1:E:377:TRP:HE1	1:E:384:LEU:HD22	1.75	0.51
1:A:31:GLU:OE1	1:A:56:ARG:HD3	2.10	0.51
1:B:638:LEU:O	1:B:739:ARG:NH2	2.44	0.51
1:C:306:ASP:O	1:C:309:TRP:HD1	1.94	0.51
1:C:352:GLN:HA	1:C:357:PHE:CD2	2.46	0.51
1:E:282:ASP:HA	1:E:324:THR:CG2	2.40	0.51
1:E:698:GLU:OE1	1:E:715:LYS:HD3	2.09	0.51
1:B:747:LEU:HD22	1:B:750:GLY:O	2.11	0.51
1:E:463:LEU:O	1:E:477:VAL:CG1	2.52	0.51
1:A:18:HIS:O	1:A:38:PRO:HA	2.10	0.51
1:D:689:HIS:ND1	1:D:739:ARG:NE	2.53	0.51
1:E:306:ASP:O	1:E:309:TRP:HD1	1.93	0.51
1:A:122:PHE:C	1:A:123:LEU:HD22	2.31	0.51
1:B:31:GLU:HG2	1:B:58:PHE:HB3	1.91	0.51
1:B:744:VAL:HG23	1:B:772:LEU:HA	1.93	0.51
1:A:630:LEU:O	1:A:647:SER:N	2.43	0.51
1:B:17:ILE:HG13	1:B:53:PHE:HZ	1.75	0.51
1:A:635:TRP:CZ3	1:A:664:ARG:HG2	2.46	0.51
1:A:748:GLN:HB2	1:A:769:THR:HG22	1.91	0.51
1:E:150:MET:HB3	1:E:237:LEU:HB2	1.92	0.51
1:E:497:GLY:O	1:E:500:ILE:HG22	2.11	0.51
1:F:134:VAL:O	1:F:135:LYS:HB2	2.11	0.51
1:F:521:ALA:HB3	5:F:3055:HOH:O	2.10	0.51
1:F:652:GLN:NE2	1:F:654:HIS:NE2	2.59	0.51
1:D:547:VAL:HG23	1:D:550:ALA:CB	2.33	0.51
1:F:276:SER:HB2	1:F:279:THR:OG1	2.10	0.51
1:A:310:MET:SD	1:A:316:CYS:HA	2.51	0.51
1:B:274:THR:HG23	1:B:304:HIS:HD2	1.76	0.51
1:C:515:PHE:CD1	1:C:516:GLU:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:VAL:O	1:E:135:LYS:HB2	2.11	0.51
1:E:20:LEU:HD12	1:E:38:PRO:O	2.11	0.51
1:F:214:GLN:HG3	1:F:435:LYS:HG2	1.93	0.51
1:A:723:ILE:O	1:A:723:ILE:HG13	2.11	0.50
1:D:293:MET:CE	1:D:300:LEU:HD23	2.41	0.50
1:E:343:CYS:HB2	1:E:412:CYS:SG	2.52	0.50
1:F:767:ALA:O	1:F:768:LEU:C	2.49	0.50
1:A:201:MET:HE1	1:A:247:PRO:CA	2.39	0.50
1:B:274:THR:CG2	1:B:275:THR:N	2.75	0.50
1:D:165:LEU:HA	1:D:197:ILE:O	2.11	0.50
1:E:287:ASN:HD21	1:E:334:ARG:HH21	1.59	0.50
1:E:293:MET:HE2	1:E:300:LEU:HD23	1.94	0.50
1:E:767:ALA:O	1:E:769:THR:HG23	2.12	0.50
1:D:123:LEU:HD23	1:D:128:ARG:HA	1.94	0.50
1:D:296:ARG:HD2	1:D:549:TRP:CE3	2.45	0.50
1:D:476:PRO:O	1:D:477:VAL:CG1	2.60	0.50
1:D:670:ALA:HB2	1:D:701:CYS:SG	2.51	0.50
1:D:380:TRP:H	1:E:49:ASP:HA	1.75	0.50
1:A:274:THR:CG2	1:A:275:THR:N	2.74	0.50
1:D:201:MET:CE	1:D:247:PRO:HB3	2.42	0.50
1:D:630:LEU:HG	1:D:635:TRP:CD1	2.46	0.50
1:D:765:GLY:C	1:D:767:ALA:H	2.13	0.50
1:E:668:LEU:O	1:E:701:CYS:HB2	2.12	0.50
1:A:735:THR:CG2	1:A:760:VAL:HG13	2.41	0.50
1:B:671:LEU:HD13	1:B:689:HIS:HD2	1.77	0.50
1:B:723:ILE:O	1:B:723:ILE:HG13	2.10	0.50
1:D:378:ASP:HA	1:D:381:GLN:O	2.11	0.50
1:A:380:TRP:CD1	1:A:381:GLN:HG2	2.47	0.50
1:B:332:ILE:HG12	1:B:408:MET:O	2.12	0.50
1:B:379:LYS:O	1:B:380:TRP:HB3	2.11	0.50
1:C:133:GLN:HB2	1:C:136:ASN:ND2	2.26	0.50
1:D:32:MET:HE1	1:D:94:ILE:HG23	1.91	0.50
1:B:20:LEU:HD12	1:B:38:PRO:O	2.11	0.50
1:B:736:LEU:C	1:B:736:LEU:HD13	2.32	0.50
1:C:725:VAL:CG2	1:C:768:LEU:HD12	2.42	0.50
1:F:748:GLN:O	1:F:768:LEU:HA	2.12	0.50
1:A:273:LEU:HD12	1:A:303:PHE:CE1	2.47	0.50
1:A:61:GLN:HB2	1:A:64:ILE:HD12	1.94	0.50
1:B:417:PHE:HA	1:B:419:GLU:OE2	2.12	0.50
1:B:548:PRO:HG3	1:B:559:VAL:HG21	1.94	0.50
1:C:654:HIS:ND1	1:C:658:SER:OG	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:THR:HG23	1:B:46:TRP:CD1	2.47	0.50
1:D:500:ILE:HG12	1:D:505:PHE:HB2	1.94	0.50
1:E:214:GLN:NE2	1:E:232:VAL:CG2	2.75	0.50
1:F:554:GLU:O	1:F:558:VAL:HG23	2.12	0.50
1:F:692:ASN:HD22	1:F:692:ASN:N	2.06	0.50
1:A:16:LEU:CD2	1:A:140:VAL:HG22	2.40	0.49
1:A:695:ASP:OD1	1:A:719:THR:O	2.29	0.49
1:C:17:ILE:HG13	1:C:53:PHE:HZ	1.76	0.49
1:D:693:LEU:HD13	1:D:718:ARG:HB2	1.94	0.49
1:E:293:MET:CE	1:E:300:LEU:HD23	2.42	0.49
1:E:38:PRO:HG2	1:E:51:PRO:HB2	1.94	0.49
1:C:747:LEU:HD22	1:C:750:GLY:O	2.12	0.49
1:D:546:ARG:N	1:D:546:ARG:HH11	2.09	0.49
1:D:588:MET:HE3	5:D:3075:HOH:O	2.12	0.49
1:D:733:ASN:OD1	1:D:733:ASN:O	2.29	0.49
1:E:489:SER:O	1:E:492:GLU:HG2	2.12	0.49
1:F:17:ILE:CG1	1:F:139:TYR:HB3	2.42	0.49
1:A:182:TRP:CE3	1:A:215:CYS:HB2	2.48	0.49
1:C:163:TYR:HB3	1:C:502:LEU:HD13	1.94	0.49
1:C:347:ASN:HA	1:C:444:TYR:OH	2.12	0.49
1:C:70:GLU:HG2	5:C:3100:HOH:O	2.11	0.49
1:D:160:GLU:HG3	1:D:204:ARG:HG2	1.94	0.49
1:D:770:ILE:N	1:D:770:ILE:HD12	2.28	0.49
1:F:579:ARG:NH1	1:F:579:ARG:HG3	2.27	0.49
1:B:525:LYS:HG2	1:B:558:VAL:HG21	1.94	0.49
1:C:123:LEU:HD13	1:C:128:ARG:HA	1.94	0.49
1:C:274:THR:HG21	1:C:540:HIS:CG	2.48	0.49
1:C:298:LEU:HD23	1:C:560:ARG:HG3	1.93	0.49
1:C:479:TRP:CZ2	3:C:803:XYF:H4	2.48	0.49
1:D:382:PRO:HG2	5:D:3059:HOH:O	2.11	0.49
1:D:576:GLU:O	1:D:579:ARG:HB2	2.13	0.49
1:D:738:LEU:HB2	1:D:741:VAL:HB	1.94	0.49
1:D:749:ASP:OD2	1:D:767:ALA:HB3	2.12	0.49
1:E:305:PHE:HB2	1:E:344:VAL:HG12	1.95	0.49
1:E:748:GLN:HB2	1:E:769:THR:OG1	2.13	0.49
1:F:219:GLU:HB2	1:F:229:GLN:HB3	1.93	0.49
1:B:447:LEU:C	1:B:447:LEU:HD23	2.33	0.49
1:B:747:LEU:HD23	1:B:748:GLN:H	1.76	0.49
1:B:723:ILE:CG1	1:B:770:ILE:HB	2.42	0.49
1:E:548:PRO:HG3	1:E:559:VAL:HG21	1.95	0.49
1:E:763:PRO:O	1:E:764:GLN:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:HIS:O	1:F:38:PRO:HA	2.13	0.49
1:F:414:LYS:NZ	1:F:538:ARG:HH22	2.10	0.49
1:A:107:ASN:ND2	1:A:125:ASN:HD21	2.05	0.49
1:A:124:ARG:NH2	1:A:243:ASP:OD1	2.43	0.49
1:A:290:ILE:HD12	1:A:335:LEU:HD22	1.95	0.49
1:A:576:GLU:HG3	1:A:611:GLY:HA3	1.93	0.49
1:E:772:LEU:HD22	1:E:772:LEU:N	2.28	0.49
1:F:438:ASN:HB3	5:F:3119:HOH:O	2.12	0.49
1:B:152:GLU:HB3	1:B:230:PHE:CE1	2.48	0.49
1:B:273:LEU:HD12	1:B:303:PHE:HE1	1.78	0.49
1:E:124:ARG:NH2	1:E:243:ASP:OD1	2.46	0.49
1:E:747:LEU:HD22	1:E:750:GLY:O	2.13	0.49
1:A:417:PHE:HA	1:A:419:GLU:OE2	2.12	0.49
1:A:262:ALA:HB3	1:A:476:PRO:HG3	1.94	0.49
1:B:332:ILE:O	1:B:336:LYS:HG3	2.13	0.49
1:C:670:ALA:C	1:C:671:LEU:HD12	2.33	0.49
1:D:698:GLU:OE1	1:D:715:LYS:HD3	2.13	0.49
1:F:134:VAL:HG22	1:F:135:LYS:HG3	1.95	0.49
1:A:453:LYS:HG3	1:A:458:GLU:HG3	1.93	0.49
1:C:668:LEU:CD2	1:C:714:LEU:HD12	2.32	0.49
1:E:736:LEU:HD13	1:E:736:LEU:C	2.33	0.49
1:F:82:TYR:HB3	1:F:84:LEU:HD13	1.95	0.49
1:A:58:PHE:N	1:A:58:PHE:CD1	2.81	0.48
1:C:356:VAL:HG11	1:C:397:TRP:CH2	2.48	0.48
1:C:652:GLN:NE2	1:C:654:HIS:NE2	2.60	0.48
1:D:145:ASN:OD1	1:D:147:ARG:HB2	2.13	0.48
1:F:719:THR:HG22	5:F:3140:HOH:O	2.13	0.48
1:A:498:LEU:HD21	1:A:608:TYR:HB3	1.95	0.48
1:B:204:ARG:HD2	1:B:206:TYR:HE2	1.79	0.48
1:C:82:TYR:HB2	1:C:84:LEU:CD2	2.42	0.48
1:E:723:ILE:CG1	1:E:770:ILE:HB	2.41	0.48
1:A:749:ASP:HB3	1:A:764:GLN:O	2.13	0.48
1:B:16:LEU:CD2	1:B:140:VAL:HG22	2.43	0.48
1:B:748:GLN:HG3	1:B:769:THR:HB	1.94	0.48
1:D:273:LEU:C	1:D:273:LEU:HD13	2.33	0.48
1:D:273:LEU:HD12	1:D:303:PHE:HD1	1.77	0.48
1:D:723:ILE:CG1	1:D:770:ILE:HB	2.43	0.48
1:E:277:PHE:CD2	1:E:278:THR:HG23	2.48	0.48
1:B:134:VAL:O	1:B:135:LYS:HB2	2.13	0.48
1:B:432:ASP:OD2	1:B:435:LYS:HG3	2.13	0.48
1:E:201:MET:CE	1:E:247:PRO:HA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ASN:HA	1:B:444:TYR:OH	2.14	0.48
1:C:208:VAL:HA	1:C:240:PHE:O	2.13	0.48
1:C:2:LYS:HA	1:C:223:GLU:OE1	2.13	0.48
1:E:634:ARG:NH2	1:E:634:ARG:HG3	2.28	0.48
1:F:280:ASN:HB3	5:F:3086:HOH:O	2.13	0.48
1:F:336:LYS:HG2	1:F:342:ILE:HD13	1.94	0.48
1:C:500:ILE:HG12	1:C:505:PHE:HB2	1.95	0.48
1:C:692:ASN:ND2	1:C:692:ASN:N	2.61	0.48
1:D:515:PHE:CD1	1:D:542:SER:HB2	2.49	0.48
1:D:719:THR:CG2	1:D:722:THR:HB	2.44	0.48
1:E:208:VAL:HA	1:E:240:PHE:O	2.13	0.48
1:F:522:HIS:CB	1:F:622:GLU:HG3	2.44	0.48
1:A:405:LEU:O	1:A:408:MET:HB3	2.14	0.48
1:B:296:ARG:HD3	1:B:556:CYS:SG	2.53	0.48
1:B:332:ILE:HD12	1:B:332:ILE:C	2.34	0.48
1:B:672:GLY:HA3	1:B:680:TYR:OH	2.13	0.48
1:C:11:GLN:HB2	1:C:14:LEU:HD12	1.96	0.48
1:D:274:THR:OG1	1:D:304:HIS:HB3	2.14	0.48
1:D:315:TRP:CE3	1:D:381:GLN:NE2	2.82	0.48
1:D:580:ALA:HA	1:D:585:THR:O	2.14	0.48
1:E:282:ASP:HB3	1:E:324:THR:HG23	1.94	0.48
1:E:300:LEU:HD13	1:E:301:HIS:N	2.28	0.48
1:F:136:ASN:HB3	1:F:153:ARG:HB2	1.96	0.48
1:A:121:ASP:OD1	1:A:128:ARG:HD2	2.14	0.48
1:C:540:HIS:C	1:C:546:ARG:HG3	2.34	0.48
1:D:164:GLY:O	1:D:165:LEU:HB2	2.14	0.48
1:D:327:ASP:OD2	1:D:330:GLY:HA3	2.14	0.48
1:D:540:HIS:C	1:D:546:ARG:NE	2.63	0.48
1:D:725:VAL:CB	1:D:768:LEU:HD12	2.40	0.48
1:E:274:THR:CG2	1:E:275:THR:N	2.77	0.48
1:F:333:ARG:HH11	1:F:333:ARG:HG2	1.78	0.48
1:F:332:ILE:O	1:F:336:LYS:HG3	2.13	0.48
1:F:515:PHE:CD1	1:F:542:SER:HB2	2.49	0.48
1:A:31:GLU:HG2	1:A:58:PHE:HB3	1.94	0.48
1:B:670:ALA:HB2	1:B:701:CYS:SG	2.54	0.48
1:C:272:TRP:HB2	1:C:538:ARG:HG3	1.94	0.48
1:C:272:TRP:CB	1:C:538:ARG:HG3	2.44	0.48
1:D:136:ASN:HD21	1:D:227:LYS:HE2	1.77	0.48
1:E:466:ARG:HB2	1:E:479:TRP:CZ3	2.48	0.48
1:F:277:PHE:HB3	1:F:542:SER:O	2.14	0.48
1:D:698:GLU:HG3	1:D:717:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:TYR:CD2	1:E:113:SER:HA	2.49	0.48
1:F:262:ALA:HB3	1:F:476:PRO:HG3	1.95	0.48
1:B:521:ALA:O	1:B:525:LYS:HD3	2.13	0.47
1:B:693:LEU:HD21	1:B:697:HIS:O	2.14	0.47
1:C:579:ARG:NH1	1:C:579:ARG:CG	2.76	0.47
1:C:772:LEU:N	1:C:772:LEU:HD22	2.29	0.47
1:D:273:LEU:HD12	1:D:303:PHE:CD1	2.49	0.47
1:D:748:GLN:O	1:D:768:LEU:HA	2.14	0.47
1:E:588:MET:HG3	1:E:608:TYR:CD1	2.48	0.47
1:F:290:ILE:HD11	1:F:335:LEU:HD22	1.96	0.47
1:B:766:ASN:O	1:B:767:ALA:CB	2.62	0.47
1:E:283:GLU:OE2	1:E:331:MET:HB2	2.14	0.47
1:A:167:GLU:OE2	1:A:195:LYS:NZ	2.45	0.47
1:A:267:TRP:CE3	1:A:341:LYS:HG3	2.49	0.47
1:B:476:PRO:C	1:B:477:VAL:HG12	2.34	0.47
1:B:753:ALA:O	1:B:759:LEU:HD12	2.13	0.47
1:E:133:GLN:HB2	1:E:136:ASN:ND2	2.29	0.47
1:E:43:GLU:HB3	1:E:45:THR:HG22	1.96	0.47
1:C:274:THR:HG23	1:C:276:SER:H	1.79	0.47
1:E:731:ALA:O	1:E:732:LYS:HD2	2.15	0.47
1:F:17:ILE:HG13	1:F:53:PHE:HZ	1.80	0.47
1:B:273:LEU:HB2	1:B:300:LEU:HD11	1.95	0.47
1:A:191:GLU:HB3	1:D:222:SER:O	2.15	0.47
1:F:515:PHE:HE2	1:F:540:HIS:HE2	1.63	0.47
1:A:261:PRO:HA	1:A:473:GLN:O	2.14	0.47
1:A:692:ASN:HD22	1:A:692:ASN:N	2.10	0.47
1:B:277:PHE:HB3	1:B:542:SER:O	2.15	0.47
1:D:405:LEU:O	1:D:408:MET:HB3	2.15	0.47
1:D:437:HIS:HB3	5:D:3049:HOH:O	2.13	0.47
1:E:298:LEU:HD13	1:E:548:PRO:HG2	1.96	0.47
1:F:659:LEU:O	1:F:661:VAL:HG23	2.14	0.47
1:F:735:THR:CG2	1:F:760:VAL:HG13	2.45	0.47
1:A:479:TRP:CZ2	3:A:801:XYF:H4	2.48	0.47
1:C:20:LEU:HD22	1:C:134:VAL:HG22	1.97	0.47
1:D:746:GLY:N	1:D:771:THR:HG23	2.30	0.47
1:A:201:MET:CE	1:A:247:PRO:HA	2.45	0.47
1:A:512:ILE:HA	1:A:527:TRP:CD1	2.50	0.47
1:B:509:SER:HB2	1:B:536:HIS:HB2	1.97	0.47
1:E:191:GLU:HB3	1:F:222:SER:O	2.14	0.47
1:A:497:GLY:O	1:A:500:ILE:HG22	2.14	0.47
1:A:692:ASN:ND2	1:A:692:ASN:H	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:THR:HG21	1:B:540:HIS:CE1	2.49	0.47
1:C:267:TRP:CE3	1:C:341:LYS:HG3	2.49	0.47
1:D:356:VAL:HG12	1:D:360:LEU:HG	1.96	0.47
1:D:772:LEU:N	1:D:772:LEU:HD22	2.30	0.47
1:B:273:LEU:HD12	1:B:303:PHE:CE1	2.50	0.47
1:C:772:LEU:HD22	1:C:772:LEU:H	1.80	0.47
1:E:290:ILE:HD12	1:E:335:LEU:HD22	1.96	0.47
1:E:80:PRO:HD3	1:E:431:SER:HB3	1.96	0.47
1:B:64:ILE:HG12	1:B:242:ILE:HG23	1.97	0.46
1:C:747:LEU:HD23	1:C:748:GLN:N	2.29	0.46
1:C:510:HIS:CD2	1:C:510:HIS:N	2.82	0.46
1:D:634:ARG:HH21	1:D:634:ARG:HG3	1.80	0.46
1:F:687:ALA:O	1:F:689:HIS:HD2	1.98	0.46
1:A:123:LEU:HD22	1:A:123:LEU:N	2.31	0.46
1:A:749:ASP:C	1:A:764:GLN:HB2	2.36	0.46
1:B:364:GLY:HA2	5:B:3104:HOH:O	2.15	0.46
1:D:560:ARG:O	1:D:564:GLN:HG3	2.16	0.46
1:E:296:ARG:HG3	1:E:296:ARG:HH11	1.80	0.46
1:E:634:ARG:HH21	1:E:634:ARG:HG3	1.79	0.46
1:F:32:MET:HE2	1:F:101:ALA:HB1	1.96	0.46
1:A:352:GLN:HA	1:A:357:PHE:CD2	2.50	0.46
1:B:610:LEU:O	1:B:614:VAL:HG13	2.15	0.46
1:C:745:ASN:HB3	1:C:771:THR:O	2.16	0.46
1:E:300:LEU:HD12	1:E:340:LEU:HD22	1.97	0.46
1:E:472:ALA:HB1	5:E:3063:HOH:O	2.15	0.46
1:A:70:GLU:HG3	5:A:3171:HOH:O	2.16	0.46
1:A:761:VAL:CG1	1:A:768:LEU:HD21	2.43	0.46
1:B:44:ARG:HA	1:B:47:GLN:CG	2.42	0.46
1:C:766:ASN:O	1:C:767:ALA:HB2	2.15	0.46
1:D:389:PHE:O	1:D:395:CYS:SG	2.73	0.46
1:F:735:THR:CG2	1:F:736:LEU:N	2.78	0.46
1:C:17:ILE:O	1:C:17:ILE:HG13	2.14	0.46
1:F:747:LEU:HD23	1:F:748:GLN:N	2.31	0.46
1:B:341:LYS:O	1:B:342:ILE:HD12	2.15	0.46
1:B:525:LYS:O	1:B:528:CYS:HB2	2.16	0.46
1:D:278:THR:CG2	1:E:45:THR:HA	2.45	0.46
1:F:275:THR:O	1:F:276:SER:CB	2.62	0.46
1:A:273:LEU:C	1:A:273:LEU:HD13	2.36	0.46
1:A:693:LEU:HD22	1:A:718:ARG:HB3	1.97	0.46
1:B:82:TYR:CD1	1:B:470:VAL:HB	2.50	0.46
1:D:479:TRP:CZ3	1:D:481:GLY:HA2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ILE:HD13	1:A:340:LEU:CD1	2.46	0.46
1:C:452:LEU:HA	1:C:452:LEU:HD12	1.76	0.46
1:D:738:LEU:CB	1:D:741:VAL:HB	2.46	0.46
1:E:41:VAL:C	1:E:43:GLU:H	2.18	0.46
1:F:525:LYS:HD3	1:F:656:PHE:CG	2.51	0.46
1:C:693:LEU:HD13	1:C:718:ARG:HB2	1.98	0.46
1:E:129:ILE:O	1:E:130:THR:HB	2.15	0.46
1:C:44:ARG:HB3	1:E:308:PHE:CZ	2.51	0.46
1:F:201:MET:HE3	1:F:247:PRO:HB3	1.98	0.46
1:B:137:ASN:HB3	1:B:152:GLU:OE1	2.15	0.45
1:B:331:MET:O	1:B:335:LEU:HG	2.16	0.45
1:C:167:GLU:OE2	1:C:195:LYS:NZ	2.43	0.45
1:C:262:ALA:HB3	1:C:476:PRO:HG3	1.97	0.45
1:C:84:LEU:N	1:C:84:LEU:HD22	2.31	0.45
1:E:248:LYS:HB2	2:E:3006:SO4:O4	2.16	0.45
1:E:287:ASN:ND2	1:E:334:ARG:HH21	2.14	0.45
1:F:569:MET:CB	1:F:573:LEU:HD22	2.46	0.45
1:A:719:THR:HG23	1:A:720:GLY:N	2.31	0.45
1:B:304:HIS:HA	1:B:343:CYS:O	2.17	0.45
1:B:717:ALA:O	1:B:723:ILE:HA	2.15	0.45
1:C:588:MET:HE3	5:C:3030:HOH:O	2.17	0.45
1:D:297:ASN:O	1:D:299:PRO:HD3	2.16	0.45
1:D:269:PHE:O	1:D:566:LYS:HE2	2.15	0.45
1:E:129:ILE:HG22	1:E:204:ARG:NH1	2.30	0.45
1:E:32:MET:HE1	1:E:101:ALA:HB1	1.97	0.45
1:E:348:PRO:HG2	1:E:349:TYR:CE1	2.51	0.45
1:E:48:LEU:HD12	1:E:49:ASP:OD2	2.16	0.45
1:F:289:PHE:CD1	1:F:547:VAL:HG11	2.51	0.45
1:C:425:VAL:HG22	1:C:426:GLN:H	1.68	0.45
1:A:176:GLY:O	1:D:177:GLN:HB3	2.16	0.45
1:D:205:GLY:HA3	1:D:245:PRO:O	2.15	0.45
1:D:719:THR:HG23	1:D:720:GLY:N	2.32	0.45
1:E:136:ASN:HB3	1:E:153:ARG:HB2	1.98	0.45
1:F:201:MET:CE	1:F:247:PRO:HB3	2.47	0.45
1:F:500:ILE:HG12	1:F:505:PHE:HB2	1.98	0.45
1:F:746:GLY:H	1:F:771:THR:HG23	1.82	0.45
1:A:267:TRP:CD2	1:A:341:LYS:HG3	2.51	0.45
1:C:267:TRP:CD2	1:C:341:LYS:HG3	2.52	0.45
1:C:48:LEU:HD23	1:C:48:LEU:N	2.31	0.45
1:C:525:LYS:HD2	1:C:555:SER:HA	1.99	0.45
1:C:736:LEU:C	1:C:736:LEU:HD13	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ARG:HG2	1:D:229:GLN:HB2	1.99	0.45
1:D:262:ALA:HB3	1:D:476:PRO:CG	2.44	0.45
1:E:165:LEU:HD13	1:E:179:VAL:CG1	2.38	0.45
1:E:282:ASP:HA	1:E:324:THR:HG23	1.98	0.45
1:F:732:LYS:N	1:F:732:LYS:HD2	2.30	0.45
1:A:681:VAL:HG22	1:A:681:VAL:O	2.17	0.45
1:A:735:THR:HG23	1:A:760:VAL:HG13	1.97	0.45
1:C:137:ASN:HB3	1:C:152:GLU:OE1	2.17	0.45
1:D:447:LEU:C	1:D:447:LEU:HD23	2.37	0.45
1:C:277:PHE:CZ	1:D:48:LEU:HD22	2.52	0.45
1:D:549:TRP:HB3	1:D:556:CYS:SG	2.56	0.45
1:E:291:ASP:O	1:E:295:GLU:HG3	2.17	0.45
1:E:654:HIS:N	1:E:654:HIS:CD2	2.85	0.45
1:F:60:PRO:O	1:F:61:GLN:HG3	2.16	0.45
1:F:570:MET:HG3	1:F:678:PRO:HA	1.97	0.45
1:A:123:LEU:HD13	1:A:128:ARG:CA	2.47	0.45
1:A:425:VAL:CG2	1:A:426:GLN:N	2.79	0.45
1:A:767:ALA:O	1:A:768:LEU:C	2.54	0.45
1:B:327:ASP:OD2	1:B:330:GLY:HA3	2.17	0.45
1:C:671:LEU:N	1:C:671:LEU:HD12	2.32	0.45
1:C:730:GLU:HG3	1:C:732:LYS:HZ3	1.79	0.45
1:F:476:PRO:C	1:F:477:VAL:HG12	2.37	0.45
1:A:155:ASP:OD1	1:A:227:LYS:HE3	2.16	0.45
1:A:274:THR:CG2	1:A:276:SER:H	2.05	0.45
1:A:264:PRO:HD3	1:A:507:PHE:CE2	2.52	0.45
1:A:723:ILE:O	1:A:723:ILE:CG1	2.65	0.45
1:A:731:ALA:C	1:A:732:LYS:HD2	2.37	0.45
1:B:671:LEU:CD1	1:B:671:LEU:N	2.80	0.45
1:D:163:TYR:HB3	1:D:502:LEU:HD13	1.98	0.45
1:D:736:LEU:HD13	1:D:737:CYS:N	2.31	0.45
1:E:196:ASN:C	1:E:197:ILE:HG12	2.37	0.45
1:E:45:THR:HG23	1:E:46:TRP:CD1	2.32	0.45
1:E:752:GLN:HB2	1:E:759:LEU:HD11	1.98	0.45
1:E:190:THR:HA	1:F:223:GLU:O	2.16	0.45
1:F:329:GLU:H	1:F:329:GLU:CD	2.20	0.45
1:F:379:LYS:O	1:F:380:TRP:HB3	2.16	0.45
1:A:689:HIS:CE1	1:A:739:ARG:HH21	2.35	0.45
1:B:466:ARG:HB2	1:B:479:TRP:CH2	2.52	0.45
1:F:510:HIS:CD2	1:F:510:HIS:N	2.83	0.45
1:A:693:LEU:HD11	1:A:716:ALA:O	2.17	0.45
1:B:277:PHE:CD2	1:B:278:THR:HG23	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:718:ARG:HB2	1:E:723:ILE:CG2	2.46	0.45
1:F:538:ARG:NH2	1:F:540:HIS:CD2	2.85	0.45
1:F:692:ASN:ND2	1:F:692:ASN:N	2.64	0.45
1:A:290:ILE:HD13	1:A:340:LEU:HD11	1.98	0.45
1:B:703:VAL:O	1:B:711:ILE:HG22	2.17	0.45
1:C:273:LEU:HD13	1:C:273:LEU:C	2.37	0.45
1:C:347:ASN:ND2	1:C:349:TYR:H	2.14	0.45
1:C:466:ARG:HB2	1:C:479:TRP:CH2	2.52	0.45
1:C:692:ASN:ND2	5:C:3050:HOH:O	2.48	0.45
1:E:297:ASN:O	1:E:299:PRO:HD3	2.16	0.45
1:F:690:LEU:HD21	1:F:693:LEU:HD12	1.99	0.45
1:A:476:PRO:O	1:A:477:VAL:HG13	2.17	0.44
1:C:630:LEU:O	1:C:647:SER:N	2.50	0.44
1:D:201:MET:HE1	1:D:247:PRO:HB3	1.99	0.44
1:D:276:SER:HB2	1:D:279:THR:CG2	2.47	0.44
1:D:38:PRO:HG2	1:D:51:PRO:HD2	1.98	0.44
1:E:731:ALA:C	1:E:732:LYS:HD2	2.37	0.44
1:F:82:TYR:CD1	1:F:470:VAL:HB	2.52	0.44
1:F:634:ARG:NH2	1:F:643:GLU:CB	2.80	0.44
1:B:272:TRP:HB2	1:B:538:ARG:HA	1.98	0.44
1:D:278:THR:HG21	1:E:45:THR:HA	1.98	0.44
1:C:277:PHE:HZ	1:D:48:LEU:HD22	1.81	0.44
1:E:262:ALA:HB3	1:E:476:PRO:CG	2.47	0.44
1:B:247:PRO:HD2	5:B:3046:HOH:O	2.16	0.44
1:C:24:GLU:HA	2:C:3011:SO4:O1	2.17	0.44
1:C:279:THR:HG22	1:C:543:LYS:O	2.17	0.44
1:C:498:LEU:HD21	1:C:608:TYR:HB3	1.99	0.44
1:F:89:ASP:N	1:F:89:ASP:OD1	2.49	0.44
1:B:631:PRO:HD2	1:B:635:TRP:CZ2	2.52	0.44
1:C:482:ASP:OD1	3:C:803:XYF:O4	2.33	0.44
1:D:100:TYR:HE2	1:D:113:SER:HG	1.64	0.44
1:D:275:THR:O	1:D:275:THR:HG23	2.17	0.44
1:B:191:GLU:HB3	1:C:222:SER:O	2.17	0.44
1:B:635:TRP:CZ3	1:B:664:ARG:HG2	2.53	0.44
1:C:576:GLU:O	1:C:579:ARG:HB3	2.16	0.44
1:D:635:TRP:CH2	1:D:664:ARG:HG2	2.52	0.44
1:F:342:ILE:HD12	1:F:342:ILE:N	2.33	0.44
1:F:353:LYS:HG2	1:F:353:LYS:O	2.17	0.44
1:F:551:TYR:O	1:F:552:ASP:HB3	2.18	0.44
1:F:252:ASP:HA	1:F:583:ARG:O	2.17	0.44
1:F:619:VAL:HG11	1:F:624:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:GLN:O	1:A:749:ASP:HB2	2.17	0.44
1:C:100:TYR:CD1	1:C:111:ARG:HD2	2.53	0.44
1:D:341:LYS:C	1:D:342:ILE:HD12	2.38	0.44
1:D:348:PRO:HG2	1:D:349:TYR:CE1	2.53	0.44
1:D:744:VAL:HG21	1:D:770:ILE:CG2	2.47	0.44
1:D:749:ASP:CG	1:D:767:ALA:HB3	2.38	0.44
1:F:45:THR:HG23	1:F:46:TRP:CD1	2.53	0.44
1:F:692:ASN:H	1:F:692:ASN:ND2	2.12	0.44
1:A:137:ASN:HB3	1:A:152:GLU:OE1	2.17	0.44
1:A:38:PRO:HG2	1:A:51:PRO:HD2	1.99	0.44
1:B:668:LEU:O	1:B:701:CYS:HB2	2.18	0.44
1:B:751:SER:OG	1:B:762:LYS:HB3	2.18	0.44
1:D:488:GLU:O	1:D:492:GLU:HG3	2.16	0.44
1:A:11:GLN:HB2	1:A:14:LEU:HD12	2.00	0.44
1:A:711:ILE:O	1:A:711:ILE:HG12	2.17	0.44
1:B:2:LYS:HA	1:B:223:GLU:OE1	2.18	0.44
1:D:452:LEU:HD12	1:D:452:LEU:N	2.33	0.44
1:D:610:LEU:O	1:D:614:VAL:HG13	2.17	0.44
1:F:347:ASN:HA	1:F:444:TYR:OH	2.18	0.44
1:A:290:ILE:HD12	1:A:335:LEU:CD2	2.48	0.44
1:B:201:MET:HE3	1:B:247:PRO:HB3	2.00	0.44
1:B:98:GLU:H	1:B:98:GLU:CD	2.21	0.44
1:C:156:LEU:HD11	1:C:228:VAL:HG23	1.98	0.44
1:D:69:ILE:HG12	1:D:150:MET:HE1	1.99	0.44
1:D:300:LEU:HD13	1:D:301:HIS:H	1.82	0.44
1:E:489:SER:HA	1:E:492:GLU:CD	2.38	0.44
1:E:490:MET:HE3	1:E:620:PHE:CD1	2.53	0.44
1:E:744:VAL:HG23	1:E:772:LEU:HA	2.00	0.44
1:B:380:TRP:CD1	1:B:381:GLN:HG2	2.53	0.43
1:E:631:PRO:HD2	1:E:635:TRP:CZ2	2.53	0.43
1:A:273:LEU:HB2	1:A:300:LEU:HD21	2.00	0.43
1:A:744:VAL:HG22	1:A:745:ASN:N	2.32	0.43
1:B:25:VAL:HG21	1:B:114:LYS:HE2	2.00	0.43
1:B:635:TRP:CH2	1:B:664:ARG:HG2	2.53	0.43
1:C:122:PHE:C	1:C:123:LEU:HD22	2.39	0.43
1:D:735:THR:HG21	1:D:760:VAL:HG13	1.99	0.43
1:E:734:TRP:CH2	1:E:763:PRO:HG3	2.53	0.43
1:F:214:GLN:HG3	1:F:435:LYS:CG	2.48	0.43
1:A:763:PRO:HB3	1:A:768:LEU:HD12	1.99	0.43
1:C:11:GLN:HB2	1:C:14:LEU:CD1	2.48	0.43
1:C:325:PHE:N	1:C:326:PRO:HD3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:TYR:HB3	1:E:502:LEU:HD13	2.01	0.43
1:E:554:GLU:O	1:E:558:VAL:HG23	2.17	0.43
1:F:82:TYR:CB	1:F:84:LEU:HD13	2.47	0.43
1:A:25:VAL:HG21	1:A:114:LYS:HE2	2.00	0.43
1:A:327:ASP:OD2	1:A:330:GLY:HA3	2.19	0.43
1:B:532:LEU:O	1:B:566:LYS:HD2	2.18	0.43
1:F:359:GLU:OE2	1:F:363:LYS:NZ	2.49	0.43
1:A:300:LEU:HD12	1:A:340:LEU:CD2	2.48	0.43
1:A:347:ASN:ND2	1:A:349:TYR:H	2.16	0.43
1:B:575:ARG:O	1:B:578:ALA:HB3	2.18	0.43
1:C:165:LEU:HD13	1:C:179:VAL:CG2	2.48	0.43
1:C:89:ASP:N	1:C:89:ASP:OD1	2.51	0.43
1:D:522:HIS:CD2	1:D:622:GLU:HG3	2.53	0.43
1:A:425:VAL:HG22	1:A:426:GLN:H	1.81	0.43
1:D:311:LYS:HE3	1:D:314:GLN:OE1	2.18	0.43
1:E:17:ILE:HG13	1:E:17:ILE:O	2.19	0.43
1:B:516:GLU:O	1:B:517:ASN:HB2	2.19	0.43
1:C:575:ARG:CZ	1:C:579:ARG:HH12	2.31	0.43
1:D:290:ILE:CD1	1:D:335:LEU:HD22	2.49	0.43
1:E:128:ARG:HH22	1:E:131:GLY:CA	2.31	0.43
1:E:165:LEU:HA	1:E:197:ILE:O	2.18	0.43
1:F:509:SER:HB2	1:F:536:HIS:HB2	2.00	0.43
1:A:262:ALA:HB3	1:A:476:PRO:CD	2.49	0.43
1:A:429:ASP:OD1	1:A:431:SER:OG	2.30	0.43
1:A:547:VAL:HA	1:A:548:PRO:HD3	1.91	0.43
1:A:525:LYS:CG	1:A:558:VAL:HG21	2.42	0.43
1:A:751:SER:OG	1:A:762:LYS:HB3	2.19	0.43
1:C:70:GLU:HB3	1:C:236:TYR:HB2	2.01	0.43
1:D:32:MET:HB2	1:D:32:MET:HE2	1.71	0.43
1:C:48:LEU:HD13	1:E:277:PHE:HZ	1.83	0.43
1:E:588:MET:HE3	5:E:3008:HOH:O	2.19	0.43
1:F:164:GLY:O	1:F:165:LEU:HB2	2.18	0.43
1:F:275:THR:HG22	1:F:303:PHE:HZ	1.83	0.43
1:F:488:GLU:H	1:F:488:GLU:CD	2.22	0.43
1:F:479:TRP:HE1	1:F:511:ASP:CG	2.22	0.43
1:C:226:SER:O	1:C:227:LYS:HG3	2.19	0.43
1:E:164:GLY:O	1:E:165:LEU:HB2	2.18	0.43
1:E:302:VAL:HG22	1:E:341:LYS:HB2	2.00	0.43
1:E:287:ASN:ND2	1:E:334:ARG:NH2	2.64	0.43
1:A:384:LEU:C	1:A:384:LEU:HD23	2.38	0.43
1:A:476:PRO:C	1:A:477:VAL:HG13	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:PHE:HD1	1:A:516:GLU:HG2	1.84	0.43
1:A:670:ALA:HB2	1:A:701:CYS:SG	2.59	0.43
1:B:738:LEU:HD11	1:B:770:ILE:HD13	2.01	0.43
1:C:290:ILE:HD13	1:C:340:LEU:CD1	2.49	0.43
1:C:314:GLN:HB3	1:C:354:SER:HB2	2.00	0.43
1:C:525:LYS:HB3	1:C:656:PHE:CD1	2.54	0.43
1:D:576:GLU:OE2	1:D:579:ARG:NH1	2.52	0.43
1:D:765:GLY:O	1:D:767:ALA:N	2.50	0.43
1:E:310:MET:SD	1:E:316:CYS:HA	2.59	0.43
1:B:262:ALA:O	1:B:264:PRO:HD3	2.19	0.42
1:D:191:GLU:N	1:D:191:GLU:OE1	2.48	0.42
1:D:358:LYS:HE2	1:D:362:GLU:OE2	2.19	0.42
1:F:723:ILE:N	1:F:723:ILE:HD12	2.34	0.42
1:A:652:GLN:NE2	1:A:654:HIS:NE2	2.66	0.42
1:C:45:THR:HG23	1:C:46:TRP:CD1	2.53	0.42
1:C:70:GLU:OE1	1:C:73:GLN:HG2	2.18	0.42
1:D:354:SER:HA	1:D:355:PRO:HD3	1.91	0.42
1:D:264:PRO:HD3	1:D:507:PHE:CE2	2.54	0.42
1:E:318:PHE:HB2	1:E:401:LYS:HD2	2.00	0.42
1:F:406:VAL:HG11	1:F:455:THR:HB	2.01	0.42
1:F:681:VAL:HG12	2:F:3005:SO4:S	2.60	0.42
1:F:98:GLU:HG3	1:F:98:GLU:O	2.19	0.42
1:A:692:ASN:ND2	1:A:692:ASN:N	2.67	0.42
1:B:341:LYS:C	1:B:342:ILE:HD12	2.38	0.42
1:C:274:THR:HG23	1:C:276:SER:N	2.34	0.42
1:C:31:GLU:HG2	1:C:58:PHE:CB	2.49	0.42
1:D:273:LEU:HD13	1:D:274:THR:N	2.34	0.42
1:E:204:ARG:NH1	1:E:204:ARG:HG2	2.33	0.42
1:F:157:GLY:HA3	1:F:204:ARG:NH2	2.33	0.42
1:A:300:LEU:HD12	1:A:340:LEU:HD21	2.02	0.42
1:A:367:LEU:CD1	1:A:425:VAL:HG21	2.49	0.42
1:A:414:LYS:NZ	1:A:538:ARG:HH12	2.15	0.42
1:A:544:SER:O	1:A:546:ARG:NH1	2.53	0.42
1:B:201:MET:HE1	1:B:247:PRO:HB3	2.02	0.42
1:C:123:LEU:HA	1:C:127:GLU:O	2.19	0.42
1:C:212:HIS:HA	1:C:213:PRO:HD3	1.88	0.42
1:C:342:ILE:N	1:C:342:ILE:HD12	2.34	0.42
1:C:475:PHE:HA	1:C:476:PRO:HD2	1.86	0.42
1:C:748:GLN:HB2	1:C:769:THR:HB	2.01	0.42
1:D:540:HIS:CA	1:D:546:ARG:HD2	2.50	0.42
1:E:358:LYS:HG2	1:E:362:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:LYS:O	1:E:380:TRP:HB3	2.19	0.42
1:E:683:HIS:HD2	1:E:730:GLU:HG2	1.84	0.42
1:F:273:LEU:HD22	1:F:274:THR:H	1.83	0.42
1:F:691:PHE:O	1:F:692:ASN:C	2.57	0.42
1:C:341:LYS:C	1:C:342:ILE:HD12	2.40	0.42
1:C:356:VAL:HG11	1:C:397:TRP:HH2	1.85	0.42
1:D:526:ARG:HD2	1:D:619:VAL:HB	2.00	0.42
1:F:293:MET:CE	1:F:300:LEU:HD23	2.50	0.42
1:A:354:SER:HA	1:A:355:PRO:HD3	1.89	0.42
1:A:37:ALA:HA	1:A:38:PRO:HD3	1.79	0.42
1:C:43:GLU:HB3	1:C:45:THR:HG22	2.01	0.42
1:C:635:TRP:CH2	1:C:664:ARG:HB3	2.55	0.42
1:D:476:PRO:C	1:D:477:VAL:CG1	2.88	0.42
1:E:320:TRP:CE2	1:E:328:PRO:HB3	2.55	0.42
1:E:520:PRO:O	1:E:521:ALA:CB	2.67	0.42
1:F:693:LEU:HD11	1:F:716:ALA:O	2.18	0.42
1:A:320:TRP:O	1:A:322:PRO:HD3	2.20	0.42
1:A:528:CYS:O	1:A:532:LEU:HD23	2.19	0.42
1:B:123:LEU:CD2	1:B:123:LEU:N	2.82	0.42
1:B:668:LEU:CD2	1:B:714:LEU:HD12	2.29	0.42
1:C:164:GLY:O	1:C:165:LEU:HB2	2.20	0.42
1:D:69:ILE:HG12	1:D:150:MET:CE	2.50	0.42
1:D:58:PHE:N	1:D:58:PHE:CD1	2.88	0.42
1:D:619:VAL:HG11	1:D:624:GLY:HA2	2.01	0.42
1:E:58:PHE:CD1	1:E:58:PHE:N	2.88	0.42
1:E:735:THR:HG23	1:E:736:LEU:N	2.34	0.42
1:E:764:GLN:NE2	1:E:764:GLN:O	2.53	0.42
1:F:273:LEU:C	1:F:273:LEU:HD13	2.40	0.42
1:F:668:LEU:HD21	1:F:714:LEU:CD1	2.36	0.42
1:F:753:ALA:O	1:F:759:LEU:HD12	2.20	0.42
1:A:164:GLY:O	1:A:165:LEU:HB2	2.20	0.42
1:A:424:ASP:N	1:A:424:ASP:OD2	2.50	0.42
1:A:735:THR:CG2	1:A:736:LEU:N	2.81	0.42
1:B:744:VAL:CG2	1:B:772:LEU:HA	2.50	0.42
1:D:497:GLY:O	1:D:500:ILE:HG22	2.20	0.42
1:C:736:LEU:CD1	1:C:738:LEU:HD23	2.50	0.42
1:E:670:ALA:C	1:E:671:LEU:HD12	2.40	0.42
1:F:311:LYS:HE3	1:F:314:GLN:CD	2.40	0.42
1:F:80:PRO:HD3	1:F:431:SER:HB3	2.01	0.42
1:B:497:GLY:O	1:B:500:ILE:HG22	2.20	0.42
1:B:414:LYS:HZ2	1:B:538:ARG:HH12	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:TRP:CE3	1:C:215:CYS:HB2	2.55	0.42
1:C:730:GLU:HG3	1:C:732:LYS:HZ2	1.85	0.42
1:C:770:ILE:HD12	1:C:770:ILE:C	2.40	0.42
1:D:344:VAL:HG22	1:D:410:VAL:HG11	2.02	0.42
1:D:588:MET:HG3	1:D:608:TYR:CD1	2.54	0.42
1:E:17:ILE:HG12	1:E:139:TYR:HB3	2.02	0.42
1:E:334:ARG:O	1:E:337:ALA:HB3	2.20	0.42
1:E:565:LEU:O	1:E:569:MET:HG3	2.19	0.42
1:A:747:LEU:HD23	1:A:747:LEU:C	2.40	0.41
1:A:752:GLN:OE1	1:A:759:LEU:HD21	2.20	0.41
1:B:145:ASN:OD1	1:B:147:ARG:HB2	2.19	0.41
1:B:195:LYS:HB3	1:B:468:ALA:HB3	2.00	0.41
1:B:405:LEU:O	1:B:410:VAL:HG23	2.20	0.41
1:B:485:ALA:HB1	1:B:519:ALA:CB	2.48	0.41
1:B:730:GLU:HG3	1:B:732:LYS:HZ2	1.85	0.41
1:C:171:ALA:O	1:C:174:ARG:NH2	2.39	0.41
1:D:262:ALA:HB3	1:D:476:PRO:CD	2.50	0.41
1:D:634:ARG:CZ	1:D:645:ASP:OD1	2.67	0.41
1:E:214:GLN:HE22	1:E:232:VAL:HG21	1.85	0.41
1:E:314:GLN:HB3	1:E:317:ASP:OD2	2.19	0.41
1:E:37:ALA:HA	1:E:38:PRO:HD3	1.87	0.41
1:F:634:ARG:HH21	1:F:643:GLU:CB	2.24	0.41
1:A:191:GLU:OE1	1:D:223:GLU:HA	2.21	0.41
1:A:300:LEU:CD1	1:A:340:LEU:HD22	2.51	0.41
1:B:182:TRP:CE3	1:B:215:CYS:HB2	2.55	0.41
1:B:764:GLN:HG3	1:B:764:GLN:O	2.20	0.41
1:B:768:LEU:HD23	1:B:768:LEU:C	2.41	0.41
1:C:367:LEU:HD11	1:C:425:VAL:CG2	2.46	0.41
1:C:580:ALA:HA	1:C:585:THR:O	2.19	0.41
1:F:419:GLU:H	1:F:419:GLU:CD	2.23	0.41
1:B:208:VAL:HA	1:B:240:PHE:O	2.20	0.41
1:B:592:MET:C	1:B:592:MET:SD	2.98	0.41
1:B:634:ARG:HG2	1:B:692:ASN:OD1	2.20	0.41
1:C:17:ILE:HG12	1:C:139:TYR:HB3	2.02	0.41
1:C:36:ALA:O	1:C:52:LEU:HD22	2.20	0.41
1:D:21:GLN:HE22	1:D:41:VAL:H	1.68	0.41
1:E:17:ILE:CG1	1:E:139:TYR:HB3	2.51	0.41
1:F:108:LEU:HD22	1:F:243:ASP:HB2	2.02	0.41
1:F:273:LEU:HD12	1:F:303:PHE:HE1	1.85	0.41
1:F:522:HIS:CG	1:F:622:GLU:HG3	2.56	0.41
1:F:749:ASP:CG	1:F:767:ALA:HB3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:THR:HA	1:C:223:GLU:O	2.21	0.41
1:D:293:MET:HE2	1:D:300:LEU:HD23	2.02	0.41
1:D:293:MET:HE3	1:D:300:LEU:HD23	2.01	0.41
1:D:39:ARG:HD2	5:D:3056:HOH:O	2.20	0.41
1:E:547:VAL:CG2	1:E:550:ALA:HB2	2.50	0.41
1:E:296:ARG:O	1:E:560:ARG:NH1	2.54	0.41
1:E:569:MET:CB	1:E:573:LEU:HD22	2.50	0.41
1:E:634:ARG:HH21	1:E:643:GLU:HB3	1.86	0.41
1:A:273:LEU:HD12	1:A:303:PHE:HE1	1.85	0.41
1:A:308:PHE:CZ	1:B:44:ARG:HB3	2.55	0.41
1:A:307:CYS:HB3	1:A:315:TRP:CZ2	2.56	0.41
1:A:731:ALA:O	1:A:732:LYS:HD2	2.20	0.41
1:B:200:TYR:CE2	1:B:208:VAL:HG22	2.55	0.41
1:B:222:SER:O	1:C:191:GLU:HB3	2.19	0.41
1:C:526:ARG:NH2	1:C:624:GLY:HA2	2.35	0.41
1:D:745:ASN:HB3	1:D:771:THR:O	2.20	0.41
1:E:173:VAL:HG21	1:E:603:TYR:CD1	2.56	0.41
1:E:82:TYR:CD1	1:E:470:VAL:HB	2.55	0.41
1:A:336:LYS:CG	1:A:342:ILE:HD13	2.50	0.41
1:A:681:VAL:HG23	1:A:683:HIS:CE1	2.56	0.41
1:A:770:ILE:HD11	1:A:772:LEU:CD2	2.50	0.41
1:B:472:ALA:HB1	5:B:3074:HOH:O	2.21	0.41
1:B:552:ASP:OD1	1:B:555:SER:N	2.38	0.41
1:C:143:THR:O	1:C:143:THR:HG22	2.20	0.41
1:C:453:LYS:HG3	1:C:458:GLU:HA	2.02	0.41
1:C:635:TRP:CZ3	1:C:664:ARG:HB3	2.55	0.41
1:E:182:TRP:CE3	1:E:215:CYS:HB2	2.56	0.41
1:E:333:ARG:NH1	1:E:336:LYS:HE3	2.36	0.41
1:E:345:TRP:O	1:E:346:ILE:CG2	2.69	0.41
1:A:548:PRO:CG	1:A:559:VAL:HG21	2.48	0.41
1:B:252:ASP:HA	1:B:583:ARG:O	2.21	0.41
1:B:439:HIS:NE2	1:B:443:ILE:HD11	2.34	0.41
1:B:635:TRP:HB3	1:B:662:TYR:HB3	2.03	0.41
1:E:277:PHE:HB3	1:E:542:SER:HA	2.02	0.41
1:E:80:PRO:HD2	1:E:435:LYS:HB2	2.01	0.41
1:F:770:ILE:HD11	1:F:772:LEU:HD23	2.02	0.41
1:B:583:ARG:HD3	5:B:3057:HOH:O	2.19	0.41
1:B:639:TRP:HE1	1:B:640:HIS:CE1	2.38	0.41
1:B:670:ALA:C	1:B:671:LEU:HD12	2.41	0.41
1:B:718:ARG:CB	1:B:723:ILE:HG22	2.51	0.41
1:D:171:ALA:O	1:D:174:ARG:NH2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:LEU:HD12	1:D:533:LEU:HA	1.94	0.41
1:D:67:VAL:O	1:D:238:GLU:HA	2.21	0.41
1:E:275:THR:HG22	1:E:303:PHE:HZ	1.86	0.41
1:F:485:ALA:CB	1:F:519:ALA:HB2	2.31	0.41
1:E:314:GLN:HB3	1:E:354:SER:HB2	2.01	0.41
1:E:414:LYS:HZ2	1:E:538:ARG:HH12	1.69	0.41
1:F:82:TYR:CE1	1:F:470:VAL:HB	2.56	0.41
1:A:521:ALA:O	1:A:525:LYS:HE3	2.20	0.41
1:C:11:GLN:HA	1:C:12:PRO:HD3	1.97	0.41
1:E:570:MET:HG3	1:E:678:PRO:HA	2.03	0.41
1:F:212:HIS:HA	1:F:213:PRO:HD3	1.90	0.41
1:F:37:ALA:HA	1:F:38:PRO:HD3	1.81	0.41
1:F:547:VAL:HA	1:F:548:PRO:HD3	1.96	0.41
1:F:631:PRO:O	1:F:646:GLY:HA3	2.20	0.41
1:A:306:ASP:O	1:A:309:TRP:HD1	2.04	0.41
1:A:615:MET:C	1:A:615:MET:SD	3.00	0.41
1:B:633:GLY:O	1:B:646:GLY:N	2.53	0.41
1:C:37:ALA:HA	1:C:38:PRO:HD3	1.78	0.41
1:C:509:SER:OG	1:C:510:HIS:N	2.54	0.41
1:D:155:ASP:HB3	5:D:3094:HOH:O	2.21	0.41
1:E:153:ARG:HG2	1:E:229:GLN:HB2	2.02	0.41
1:E:327:ASP:OD2	1:E:330:GLY:HA3	2.20	0.41
1:E:447:LEU:O	1:E:451:VAL:HG23	2.20	0.41
1:E:716:ALA:HA	1:E:724:THR:O	2.21	0.41
1:A:11:GLN:HB2	1:A:14:LEU:CD1	2.51	0.40
1:B:120:LEU:HD23	1:B:121:ASP:N	2.36	0.40
1:C:712:PHE:CG	1:C:731:ALA:HB2	2.55	0.40
1:D:32:MET:HE3	1:D:103:PHE:HB2	2.03	0.40
1:D:261:PRO:O	1:D:581:ASN:HA	2.21	0.40
1:D:681:VAL:HG23	1:D:683:HIS:CE1	2.56	0.40
1:B:122:PHE:CE1	1:B:241:VAL:HG21	2.56	0.40
1:B:601:CYS:HA	1:B:604:LEU:HG	2.03	0.40
1:C:349:TYR:HB3	1:C:384:LEU:HD21	2.03	0.40
1:D:277:PHE:CD2	1:D:278:THR:HG23	2.56	0.40
1:D:308:PHE:CE1	1:D:315:TRP:HZ2	2.40	0.40
1:E:273:LEU:CB	1:E:300:LEU:HD21	2.48	0.40
1:E:516:GLU:O	1:E:517:ASN:CB	2.68	0.40
1:E:610:LEU:O	1:E:614:VAL:HG13	2.20	0.40
1:E:719:THR:HG22	1:E:722:THR:O	2.22	0.40
1:F:635:TRP:CZ3	1:F:664:ARG:HG2	2.56	0.40
1:F:67:VAL:O	1:F:238:GLU:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:761:VAL:HG11	1:F:768:LEU:HD11	2.03	0.40
1:A:747:LEU:HD11	1:A:761:VAL:HG13	2.02	0.40
1:B:690:LEU:O	1:B:739:ARG:HB2	2.21	0.40
1:B:718:ARG:HH21	1:B:772:LEU:HD12	1.86	0.40
1:C:18:HIS:HB2	1:C:20:LEU:CD2	2.51	0.40
1:C:310:MET:SD	1:C:316:CYS:HA	2.61	0.40
1:D:772:LEU:CD2	1:D:772:LEU:H	2.34	0.40
1:E:300:LEU:HD12	1:E:340:LEU:CD2	2.52	0.40
1:E:512:ILE:HB	1:E:539:LEU:HD23	2.02	0.40
1:B:381:GLN:O	1:B:384:LEU:HB2	2.21	0.40
1:C:274:THR:HG22	1:C:539:LEU:O	2.21	0.40
1:C:598:ASP:HA	1:C:599:PRO:HD2	1.94	0.40
1:D:282:ASP:HA	1:D:324:THR:HG23	2.04	0.40
1:D:634:ARG:NH2	1:D:634:ARG:HG3	2.35	0.40
1:F:533:LEU:HD23	1:F:659:LEU:HD11	2.03	0.40
1:F:670:ALA:HB2	1:F:701:CYS:SG	2.61	0.40
1:A:635:TRP:HB3	1:A:662:TYR:HB3	2.03	0.40
1:C:84:LEU:H	1:C:84:LEU:HD22	1.84	0.40
1:D:635:TRP:O	1:D:643:GLU:HA	2.22	0.40
1:E:324:THR:HG22	1:E:325:PHE:CE2	2.56	0.40
1:F:273:LEU:CB	1:F:300:LEU:HD21	2.45	0.40
1:F:31:GLU:OE1	1:F:56:ARG:HD3	2.22	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	771/778 (99%)	716 (93%)	45 (6%)	10 (1%)	12	9
1	B	771/778 (99%)	712 (92%)	44 (6%)	15 (2%)	8	5
1	C	771/778 (99%)	716 (93%)	47 (6%)	8 (1%)	15	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	771/778 (99%)	709 (92%)	47 (6%)	15 (2%)	8	5
1	E	771/778 (99%)	709 (92%)	52 (7%)	10 (1%)	12	9
1	F	771/778 (99%)	709 (92%)	51 (7%)	11 (1%)	11	8
All	All	4626/4668 (99%)	4271 (92%)	286 (6%)	69 (2%)	10	8

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	767	ALA
1	B	764	GLN
1	B	766	ASN
1	C	766	ASN
1	C	767	ALA
1	D	517	ASN
1	D	764	GLN
1	A	480	GLY
1	A	681	VAL
1	B	276	SER
1	B	307	CYS
1	B	308	PHE
1	B	733	ASN
1	B	772	LEU
1	C	480	GLY
1	D	276	SER
1	D	546	ARG
1	D	720	GLY
1	D	772	LEU
1	E	720	GLY
1	E	764	GLN
1	E	767	ALA
1	F	77	ASN
1	F	767	ALA
1	F	768	LEU
1	A	692	ASN
1	A	768	LEU
1	B	476	PRO
1	C	431	SER
1	D	307	CYS
1	D	476	PRO
1	D	733	ASN
1	D	767	ALA

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Mol	Chain	Res	Type
1	E	44	ARG
1	E	316	CYS
1	F	308	PHE
1	F	552	ASP
1	A	277	PHE
1	A	476	PRO
1	B	214	GLN
1	B	316	CYS
1	B	431	SER
1	B	745	ASN
1	C	316	CYS
1	C	477	VAL
1	C	764	GLN
1	D	745	ASN
1	F	276	SER
1	F	692	ASN
1	A	308	PHE
1	A	316	CYS
1	A	477	VAL
1	B	477	VAL
1	B	480	GLY
1	C	308	PHE
1	D	380	TRP
1	D	477	VAL
1	E	417	PHE
1	E	477	VAL
1	E	766	ASN
1	F	316	CYS
1	E	277	PHE
1	F	476	PRO
1	F	477	VAL
1	D	328	PRO
1	F	720	GLY
1	D	742	VAL
1	E	476	PRO
1	B	328	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	659/665 (99%)	634 (96%)	25 (4%)	33	42
1	B	659/665 (99%)	643 (98%)	16 (2%)	49	62
1	C	659/665 (99%)	630 (96%)	29 (4%)	28	35
1	D	659/665 (99%)	630 (96%)	29 (4%)	28	35
1	E	659/665 (99%)	634 (96%)	25 (4%)	33	42
1	F	659/665 (99%)	635 (96%)	24 (4%)	35	45
All	All	3954/3990 (99%)	3806 (96%)	148 (4%)	34	43

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	52	LEU
1	A	58	PHE
1	A	120	LEU
1	A	123	LEU
1	A	174	ARG
1	A	179	VAL
1	A	191	GLU
1	A	316	CYS
1	A	347	ASN
1	A	348	PRO
1	A	377	TRP
1	A	452	LEU
1	A	464	PHE
1	A	479	TRP
1	A	525	LYS
1	A	533	LEU
1	A	573	LEU
1	A	614	VAL
1	A	616	VAL
1	A	630	LEU
1	A	733	ASN
1	A	749	ASP
1	A	768	LEU
1	A	770	ILE
1	B	84	LEU
1	B	123	LEU

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Mol	Chain	Res	Type
1	B	146	GLN
1	B	179	VAL
1	B	208	VAL
1	B	227	LYS
1	B	285	THR
1	B	316	CYS
1	B	347	ASN
1	B	377	TRP
1	B	464	PHE
1	B	479	TRP
1	B	533	LEU
1	B	573	LEU
1	B	616	VAL
1	B	693	LEU
1	C	93	THR
1	C	120	LEU
1	C	123	LEU
1	C	174	ARG
1	C	179	VAL
1	C	208	VAL
1	C	276	SER
1	C	285	THR
1	C	306	ASP
1	C	316	CYS
1	C	347	ASN
1	C	348	PRO
1	C	377	TRP
1	C	452	LEU
1	C	459	GLU
1	C	464	PHE
1	C	479	TRP
1	C	510	HIS
1	C	525	LYS
1	C	533	LEU
1	C	573	LEU
1	C	579	ARG
1	C	592	MET
1	C	614	VAL
1	C	616	VAL
1	C	657	LEU
1	C	693	LEU
1	C	721	ASN

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Mol	Chain	Res	Type
1	C	770	ILE
1	D	52	LEU
1	D	69	ILE
1	D	143	THR
1	D	178	THR
1	D	179	VAL
1	D	208	VAL
1	D	289	PHE
1	D	300	LEU
1	D	306	ASP
1	D	316	CYS
1	D	347	ASN
1	D	348	PRO
1	D	352	GLN
1	D	377	TRP
1	D	459	GLU
1	D	464	PHE
1	D	477	VAL
1	D	510	HIS
1	D	527	TRP
1	D	533	LEU
1	D	537	SER
1	D	546	ARG
1	D	573	LEU
1	D	614	VAL
1	D	616	VAL
1	D	630	LEU
1	D	693	LEU
1	D	742	VAL
1	D	771	THR
1	E	45	THR
1	E	48	LEU
1	E	120	LEU
1	E	123	LEU
1	E	174	ARG
1	E	179	VAL
1	E	214	GLN
1	E	276	SER
1	E	282	ASP
1	E	300	LEU
1	E	316	CYS
1	E	377	TRP

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Mol	Chain	Res	Type
1	E	452	LEU
1	E	459	GLU
1	E	464	PHE
1	E	479	TRP
1	E	537	SER
1	E	573	LEU
1	E	614	VAL
1	E	616	VAL
1	E	630	LEU
1	E	653	GLN
1	E	723	ILE
1	E	735	THR
1	E	756	GLU
1	F	123	LEU
1	F	143	THR
1	F	174	ARG
1	F	178	THR
1	F	189	SER
1	F	214	GLN
1	F	306	ASP
1	F	316	CYS
1	F	347	ASN
1	F	348	PRO
1	F	377	TRP
1	F	452	LEU
1	F	459	GLU
1	F	464	PHE
1	F	533	LEU
1	F	537	SER
1	F	573	LEU
1	F	579	ARG
1	F	616	VAL
1	F	630	LEU
1	F	693	LEU
1	F	714	LEU
1	F	770	ILE
1	F	771	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS

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Mol	Chain	Res	Type
1	A	27	GLN
1	A	73	GLN
1	A	77	ASN
1	A	88	GLN
1	A	107	ASN
1	A	125	ASN
1	A	133	GLN
1	A	212	HIS
1	A	287	ASN
1	A	347	ASN
1	A	564	GLN
1	A	652	GLN
1	A	692	ASN
1	A	697	HIS
1	B	27	GLN
1	B	28	GLN
1	B	61	GLN
1	B	141	GLN
1	B	146	GLN
1	B	177	GLN
1	B	212	HIS
1	B	347	ASN
1	B	564	GLN
1	B	652	GLN
1	B	692	ASN
1	B	697	HIS
1	B	733	ASN
1	B	745	ASN
1	B	764	GLN
1	C	21	GLN
1	C	27	GLN
1	C	77	ASN
1	C	107	ASN
1	C	133	GLN
1	C	146	GLN
1	C	177	GLN
1	C	347	ASN
1	C	361	GLN
1	C	517	ASN
1	C	564	GLN
1	C	652	GLN
1	C	692	ASN

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Mol	Chain	Res	Type
1	C	697	HIS
1	C	721	ASN
1	C	733	ASN
1	D	7	ASN
1	D	21	GLN
1	D	27	GLN
1	D	107	ASN
1	D	133	GLN
1	D	146	GLN
1	D	381	GLN
1	D	652	GLN
1	D	697	HIS
1	D	733	ASN
1	E	11	GLN
1	E	21	GLN
1	E	27	GLN
1	E	47	GLN
1	E	73	GLN
1	E	77	ASN
1	E	107	ASN
1	E	146	GLN
1	E	192	GLN
1	E	280	ASN
1	E	652	GLN
1	E	697	HIS
1	E	733	ASN
1	E	745	ASN
1	E	764	GLN
1	F	27	GLN
1	F	73	GLN
1	F	77	ASN
1	F	107	ASN
1	F	177	GLN
1	F	280	ASN
1	F	347	ASN
1	F	652	GLN
1	F	653	GLN
1	F	692	ASN
1	F	697	HIS
1	F	733	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 ⓘ

21 ligands are modelled in this entry.

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$
2	SO4	B	3010	-	4,4,4	1.89	2 (50%)	6,6,6	0.91	0
2	SO4	F	3005	-	4,4,4	1.87	2 (50%)	6,6,6	0.89	0
2	SO4	F	3001	-	4,4,4	1.87	2 (50%)	6,6,6	0.88	0
4	MPO	C	2002	-	13,13,13	2.09	2 (15%)	17,17,17	2.23	6 (35%)
4	MPO	D	2003	-	13,13,13	1.93	2 (15%)	17,17,17	2.29	6 (35%)
2	SO4	C	3007	-	4,4,4	1.86	2 (50%)	6,6,6	0.92	0
3	XYF	C	803	1	10,10,11	1.68	3 (30%)	14,14,16	0.72	0
2	SO4	A	3013	-	4,4,4	1.89	2 (50%)	6,6,6	0.88	0
2	SO4	F	3009	-	4,4,4	1.89	2 (50%)	6,6,6	0.91	0
2	SO4	E	3006	-	4,4,4	1.89	2 (50%)	6,6,6	0.89	0
3	XYF	E	804	1	10,10,11	1.67	3 (30%)	14,14,16	0.64	0
2	SO4	D	3004	-	4,4,4	1.92	2 (50%)	6,6,6	0.90	0
4	MPO	E	2004	-	13,13,13	1.92	2 (15%)	17,17,17	2.26	6 (35%)
2	SO4	F	3002	-	4,4,4	1.87	2 (50%)	6,6,6	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	XYF	A	801	1	10,10,11	1.70	3 (30%)	14,14,16	0.67	0
2	SO4	C	3011	-	4,4,4	1.83	2 (50%)	6,6,6	0.91	0
4	MPO	B	2001	-	13,13,13	1.99	2 (15%)	17,17,17	2.28	6 (35%)
3	XYF	B	802	1	10,10,11	1.66	3 (30%)	14,14,16	0.69	0
2	SO4	B	3008	-	4,4,4	1.87	2 (50%)	6,6,6	0.91	0
2	SO4	F	3003	-	4,4,4	1.90	2 (50%)	6,6,6	0.93	0
2	SO4	A	3012	-	4,4,4	1.88	2 (50%)	6,6,6	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPO	C	2002	-	-	5/7/15/15	0/1/1/1
4	MPO	D	2003	-	-	3/7/15/15	0/1/1/1
3	XYF	C	803	1	-	-	0/1/1/1
3	XYF	B	802	1	-	-	0/1/1/1
4	MPO	E	2004	-	-	2/7/15/15	0/1/1/1
3	XYF	A	801	1	-	-	0/1/1/1
4	MPO	B	2001	-	-	3/7/15/15	0/1/1/1
3	XYF	E	804	1	-	-	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2002	MPO	C1-S1	6.24	1.86	1.77
4	B	2001	MPO	C1-S1	5.85	1.85	1.77
4	D	2003	MPO	C1-S1	5.61	1.85	1.77
4	E	2004	MPO	C1-S1	5.49	1.85	1.77
3	B	802	XYF	O5-C1	3.38	1.44	1.39
3	C	803	XYF	O5-C1	3.37	1.44	1.39
3	A	801	XYF	O5-C1	3.34	1.44	1.39
3	E	804	XYF	O5-C1	3.32	1.44	1.39
2	D	3004	SO4	O1-S	3.18	1.63	1.46
2	A	3013	SO4	O1-S	3.14	1.63	1.46
2	F	3009	SO4	O1-S	3.14	1.63	1.46
2	B	3010	SO4	O1-S	3.14	1.63	1.46
2	F	3003	SO4	O1-S	3.13	1.63	1.46
2	A	3012	SO4	O1-S	3.12	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3006	SO4	O1-S	3.12	1.62	1.46
2	B	3008	SO4	O1-S	3.11	1.62	1.46
2	F	3002	SO4	O1-S	3.10	1.62	1.46
2	F	3001	SO4	O1-S	3.09	1.62	1.46
2	F	3005	SO4	O1-S	3.09	1.62	1.46
3	E	804	XYF	F5-C1	-3.08	1.35	1.39
2	C	3007	SO4	O1-S	3.06	1.62	1.46
3	C	803	XYF	F5-C1	-3.05	1.35	1.39
3	A	801	XYF	F5-C1	-3.03	1.35	1.39
3	B	802	XYF	F5-C1	-3.03	1.35	1.39
2	C	3011	SO4	O1-S	3.01	1.62	1.46
3	A	801	XYF	C2-C1	2.66	1.53	1.52
3	C	803	XYF	C2-C1	2.51	1.53	1.52
3	E	804	XYF	C2-C1	2.45	1.53	1.52
3	B	802	XYF	C2-C1	2.39	1.53	1.52
4	B	2001	MPO	C4-N1	2.28	1.53	1.46
4	E	2004	MPO	C4-N1	2.25	1.53	1.46
4	C	2002	MPO	C4-N1	2.25	1.53	1.46
4	D	2003	MPO	C4-N1	2.14	1.52	1.46
2	F	3003	SO4	O3-S	-2.13	1.30	1.47
2	D	3004	SO4	O3-S	-2.11	1.30	1.47
2	E	3006	SO4	O3-S	-2.08	1.30	1.47
2	B	3010	SO4	O3-S	-2.08	1.30	1.47
2	A	3013	SO4	O3-S	-2.07	1.30	1.47
2	F	3005	SO4	O3-S	-2.07	1.30	1.47
2	F	3009	SO4	O3-S	-2.06	1.31	1.47
2	F	3001	SO4	O3-S	-2.06	1.31	1.47
2	F	3002	SO4	O3-S	-2.05	1.31	1.47
2	C	3007	SO4	O3-S	-2.05	1.31	1.47
2	A	3012	SO4	O3-S	-2.05	1.31	1.47
2	C	3011	SO4	O3-S	-2.05	1.31	1.47
2	B	3008	SO4	O3-S	-2.02	1.31	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2003	MPO	C2-C1-S1	-6.57	103.17	113.25
4	E	2004	MPO	C2-C1-S1	-6.42	103.41	113.25
4	B	2001	MPO	C2-C1-S1	-6.32	103.56	113.25
4	C	2002	MPO	C2-C1-S1	-6.06	103.95	113.25
4	B	2001	MPO	O1-S1-C1	3.55	111.19	106.92
4	C	2002	MPO	O1-S1-C1	3.40	111.01	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2004	MPO	O1-S1-C1	3.18	110.75	106.92
4	D	2003	MPO	O1-S1-C1	3.12	110.67	106.92
4	E	2004	MPO	O2-S1-C1	2.87	110.38	106.92
4	C	2002	MPO	O2-S1-C1	2.86	110.36	106.92
4	B	2001	MPO	O2-S1-C1	2.80	110.29	106.92
4	D	2003	MPO	O2-S1-C1	2.74	110.22	106.92
4	B	2001	MPO	C3-C2-C1	-2.40	104.76	113.14
4	D	2003	MPO	C5-C4-N1	-2.37	106.51	110.10
4	E	2004	MPO	C3-C2-C1	-2.34	104.96	113.14
4	C	2002	MPO	C5-C4-N1	-2.33	106.57	110.10
4	D	2003	MPO	C3-C2-C1	-2.31	105.06	113.14
4	E	2004	MPO	C2-C3-N1	-2.30	108.04	113.84
4	D	2003	MPO	C2-C3-N1	-2.29	108.06	113.84
4	B	2001	MPO	C2-C3-N1	-2.29	108.08	113.84
4	C	2002	MPO	C3-C2-C1	-2.28	105.17	113.14
4	C	2002	MPO	C2-C3-N1	-2.21	108.27	113.84
4	B	2001	MPO	C5-C4-N1	-2.19	106.78	110.10
4	E	2004	MPO	C5-C4-N1	-2.19	106.78	110.10

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2002	MPO	C1-C2-C3-N1
4	B	2001	MPO	C1-C2-C3-N1
4	D	2003	MPO	C2-C3-N1-C7
4	C	2002	MPO	C2-C3-N1-C4
4	C	2002	MPO	C2-C3-N1-C7
4	D	2003	MPO	C2-C3-N1-C4
4	E	2004	MPO	C2-C3-N1-C4
4	B	2001	MPO	C2-C3-N1-C4
4	E	2004	MPO	C2-C3-N1-C7
4	B	2001	MPO	C2-C3-N1-C7
4	C	2002	MPO	C2-C1-S1-O2
4	C	2002	MPO	C2-C1-S1-O3
4	D	2003	MPO	C1-C2-C3-N1

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3005	SO4	2	0
3	C	803	XYF	2	0
2	E	3006	SO4	1	0
3	E	804	XYF	2	0
3	A	801	XYF	2	0
2	C	3011	SO4	1	0
3	B	802	XYF	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	773/778 (99%)	-0.09	13 (1%)	70	68	16, 28, 48, 76	0
1	B	773/778 (99%)	0.19	46 (5%)	21	20	20, 36, 61, 82	0
1	C	773/778 (99%)	-0.06	18 (2%)	60	58	17, 29, 50, 72	0
1	D	773/778 (99%)	0.15	52 (6%)	17	16	17, 31, 63, 84	0
1	E	773/778 (99%)	-0.02	28 (3%)	42	41	18, 32, 55, 90	0
1	F	773/778 (99%)	0.11	32 (4%)	37	35	19, 30, 55, 77	0
All	All	4638/4668 (99%)	0.05	189 (4%)	37	35	16, 31, 56, 90	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	719	THR	8.8
1	B	767	ALA	8.7
1	E	46	TRP	7.8
1	B	766	ASN	7.6
1	D	382	PRO	7.3
1	F	766	ASN	7.1
1	C	766	ASN	7.0
1	D	277	PHE	6.9
1	E	43	GLU	6.8
1	E	766	ASN	6.7
1	B	765	GLY	6.3
1	D	278	THR	6.3
1	D	545	TYR	6.1
1	D	540	HIS	6.0
1	D	766	ASN	6.0
1	D	279	THR	5.9
1	E	42	ARG	5.7
1	D	765	GLY	5.2
1	E	765	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	541	GLY	5.0
1	D	546	ARG	4.9
1	A	766	ASN	4.9
1	F	765	GLY	4.9
1	C	765	GLY	4.9
1	F	748	GLN	4.8
1	D	281	TYR	4.7
1	C	767	ALA	4.6
1	B	719	THR	4.5
1	D	747	LEU	4.5
1	E	47	GLN	4.5
1	D	380	TRP	4.4
1	A	765	GLY	4.3
1	F	749	ASP	4.2
1	F	768	LEU	4.2
1	D	767	ALA	4.2
1	A	719	THR	4.1
1	C	748	GLN	4.1
1	F	770	ILE	4.1
1	D	748	GLN	4.1
1	A	768	LEU	4.0
1	B	768	LEU	4.0
1	F	772	LEU	3.9
1	B	753	ALA	3.9
1	D	764	GLN	3.9
1	F	767	ALA	3.8
1	E	767	ALA	3.8
1	E	49	ASP	3.8
1	C	770	ILE	3.8
1	D	477	VAL	3.7
1	B	744	VAL	3.6
1	B	407	ALA	3.6
1	B	722	THR	3.5
1	B	323	LEU	3.5
1	D	743	LYS	3.5
1	D	768	LEU	3.5
1	D	381	GLN	3.5
1	B	29	ASP	3.4
1	D	383	GLY	3.4
1	D	275	THR	3.4
1	D	276	SER	3.4
1	B	764	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	88	GLN	3.4
1	D	750	GLY	3.3
1	D	763	PRO	3.3
1	F	545	TYR	3.2
1	D	280	ASN	3.2
1	E	117	PHE	3.2
1	A	477	VAL	3.2
1	C	719	THR	3.2
1	E	44	ARG	3.2
1	F	724	THR	3.2
1	B	742	VAL	3.2
1	B	756	GLU	3.2
1	B	745	ASN	3.1
1	B	338	LYS	3.1
1	D	542	SER	3.1
1	A	88	GLN	3.1
1	B	738	LEU	3.1
1	D	762	LYS	3.0
1	F	88	GLN	3.0
1	B	736	LEU	3.0
1	D	753	ALA	3.0
1	B	477	VAL	3.0
1	B	295	GLU	2.9
1	B	88	GLN	2.9
1	B	325	PHE	2.9
1	D	742	VAL	2.9
1	E	40	ASP	2.9
1	D	543	LYS	2.8
1	E	477	VAL	2.8
1	B	545	TYR	2.8
1	D	745	ASN	2.8
1	F	695	ASP	2.8
1	E	41	VAL	2.8
1	B	772	LEU	2.7
1	E	45	THR	2.7
1	F	745	ASN	2.7
1	B	337	ALA	2.7
1	E	764	GLN	2.7
1	F	756	GLU	2.7
1	B	327	ASP	2.7
1	C	745	ASN	2.7
1	B	549	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	723	ILE	2.7
1	B	748	GLN	2.6
1	C	744	VAL	2.6
1	E	745	ASN	2.6
1	A	767	ALA	2.6
1	D	723	ILE	2.6
1	A	744	VAL	2.6
1	D	289	PHE	2.6
1	B	743	LYS	2.6
1	B	770	ILE	2.6
1	C	772	LEU	2.5
1	E	89	ASP	2.5
1	D	517	ASN	2.5
1	F	762	LYS	2.5
1	C	773	HIS	2.5
1	F	747	LEU	2.5
1	D	306	ASP	2.5
1	B	759	LEU	2.5
1	B	761	VAL	2.5
1	D	749	ASP	2.5
1	C	46	TRP	2.5
1	E	719	THR	2.5
1	E	706	ALA	2.4
1	F	754	GLU	2.4
1	B	333	ARG	2.4
1	C	756	GLU	2.4
1	E	723	ILE	2.4
1	E	772	LEU	2.4
1	E	98	GLU	2.4
1	F	29	ASP	2.4
1	A	721	ASN	2.4
1	C	768	LEU	2.4
1	F	771	THR	2.4
1	D	759	LEU	2.3
1	F	759	LEU	2.3
1	C	477	VAL	2.3
1	D	756	GLU	2.3
1	D	772	LEU	2.3
1	D	378	ASP	2.3
1	E	540	HIS	2.3
1	E	39	ARG	2.3
1	B	726	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	757	GLN	2.3
1	D	307	CYS	2.3
1	F	550	ALA	2.3
1	A	29	ASP	2.3
1	B	290	ILE	2.3
1	D	544	SER	2.3
1	D	88	GLN	2.3
1	D	513	GLY	2.2
1	B	30	ASN	2.2
1	C	88	GLN	2.2
1	D	514	GLY	2.2
1	C	742	VAL	2.2
1	F	547	VAL	2.2
1	E	743	LYS	2.2
1	F	746	GLY	2.2
1	F	723	ILE	2.2
1	F	515	PHE	2.2
1	A	772	LEU	2.2
1	F	738	LEU	2.2
1	B	91	LYS	2.1
1	A	742	VAL	2.1
1	F	277	PHE	2.1
1	D	483	CYS	2.1
1	B	762	LYS	2.1
1	D	377	TRP	2.1
1	B	758	GLY	2.1
1	D	333	ARG	2.1
1	B	741	VAL	2.1
1	D	741	VAL	2.1
1	A	749	ASP	2.1
1	F	764	GLN	2.1
1	B	286	VAL	2.1
1	B	721	ASN	2.1
1	E	50	THR	2.1
1	D	755	SER	2.1
1	F	742	VAL	2.1
1	B	339	GLY	2.0
1	B	204	ARG	2.0
1	D	770	ILE	2.0
1	E	76	LEU	2.0
1	F	733	ASN	2.0
1	C	764	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	750	GLY	2.0
1	C	98	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	3012	5/5	0.76	0.17	87,87,88,88	0
2	SO4	F	3001	5/5	0.77	0.20	91,91,91,92	0
2	SO4	C	3011	5/5	0.78	0.29	105,106,106,106	0
2	SO4	F	3009	5/5	0.84	0.23	91,91,92,92	0
3	XYF	B	802	10/11	0.85	0.15	37,41,43,45	0
3	XYF	C	803	10/11	0.85	0.19	33,36,38,40	0
2	SO4	B	3010	5/5	0.87	0.20	88,89,89,90	0
3	XYF	E	804	10/11	0.88	0.25	25,26,27,29	10
4	MPO	B	2001	13/13	0.88	0.17	68,68,69,69	0
4	MPO	E	2004	13/13	0.91	0.16	53,55,57,58	0
2	SO4	F	3005	5/5	0.92	0.15	58,58,59,59	0
4	MPO	C	2002	13/13	0.92	0.15	52,57,61,62	0
2	SO4	E	3006	5/5	0.93	0.17	84,84,85,85	0
3	XYF	A	801	10/11	0.93	0.10	35,36,38,39	0
2	SO4	F	3003	5/5	0.93	0.19	67,68,69,69	0
2	SO4	D	3004	5/5	0.94	0.18	75,75,75,75	0
2	SO4	A	3013	5/5	0.94	0.12	77,77,78,78	0
2	SO4	F	3002	5/5	0.94	0.16	76,77,77,78	0
4	MPO	D	2003	13/13	0.95	0.20	53,57,63,63	0
2	SO4	B	3008	5/5	0.95	0.15	72,72,72,73	0
2	SO4	C	3007	5/5	0.96	0.21	75,76,76,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.