



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:04 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

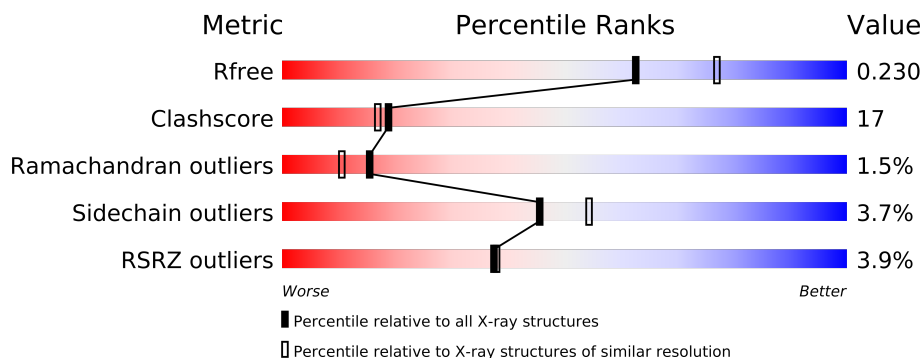
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	778	
1	B	778	
1	C	778	
1	D	778	
1	E	778	
1	F	778	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	3012	-	X
2	SO4	C	3007	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	C	3011	-	X
2	SO4	E	3006	-	X
2	SO4	F	3001	-	X
2	SO4	F	3009	-	X
3	XYF	E	804	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38360 atoms, of which 0 are hydrogen and 0 are deuterium.

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).



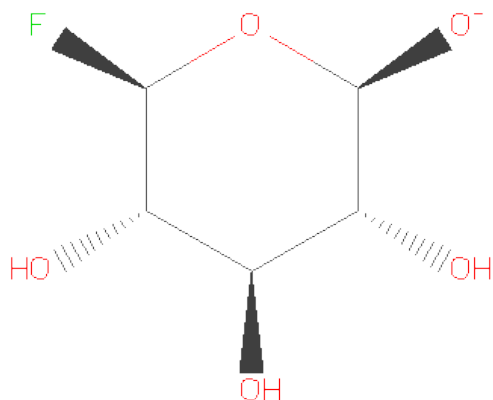
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

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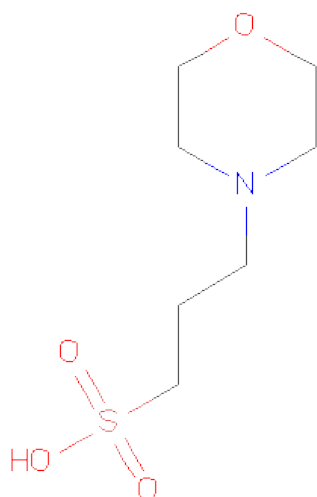
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

- Molecule 3 is 5(R)-5-FLUORO-BETA-D-XYLOPYRANOSYL-ENZYMEINTERMEDIATE (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]PROPANESULFONIC 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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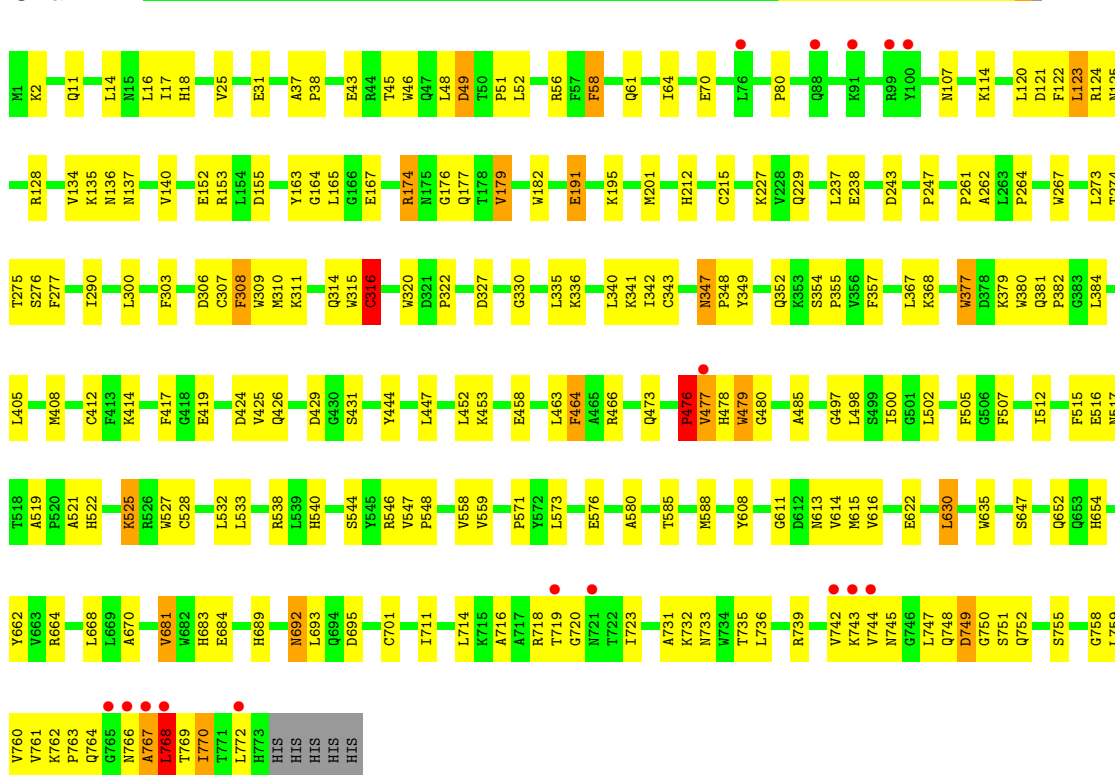
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	114	Total 114	O 114	0	0
5	C	167	Total 167	O 167	0	0
5	D	145	Total 145	O 145	0	0
5	E	122	Total 122	O 122	0	0
5	F	131	Total 131	O 131	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 family 31 glucosidase yicI

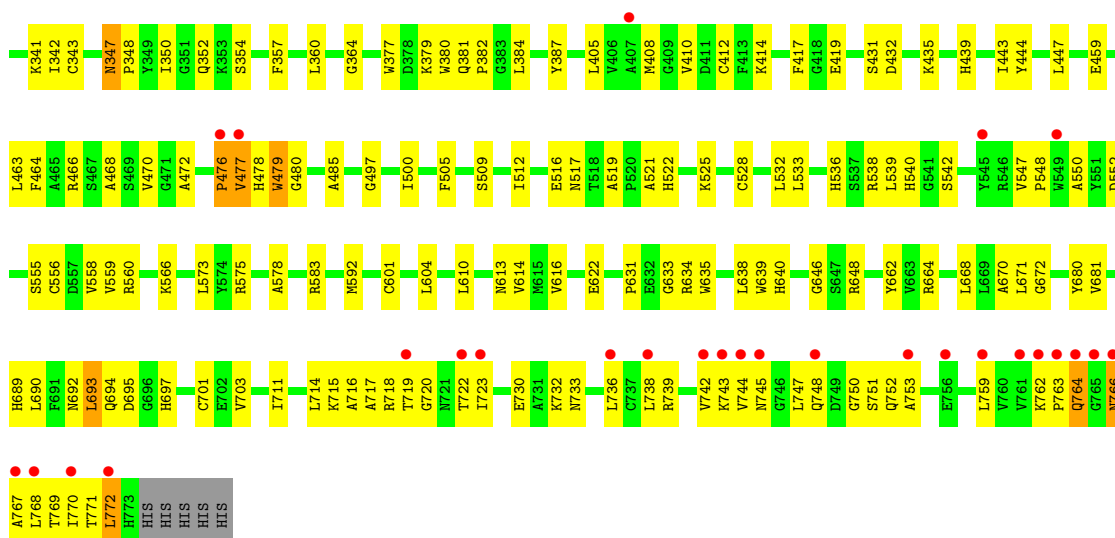
Chain A:



- Molecule 1: Putative family 31 glucosidase yicI

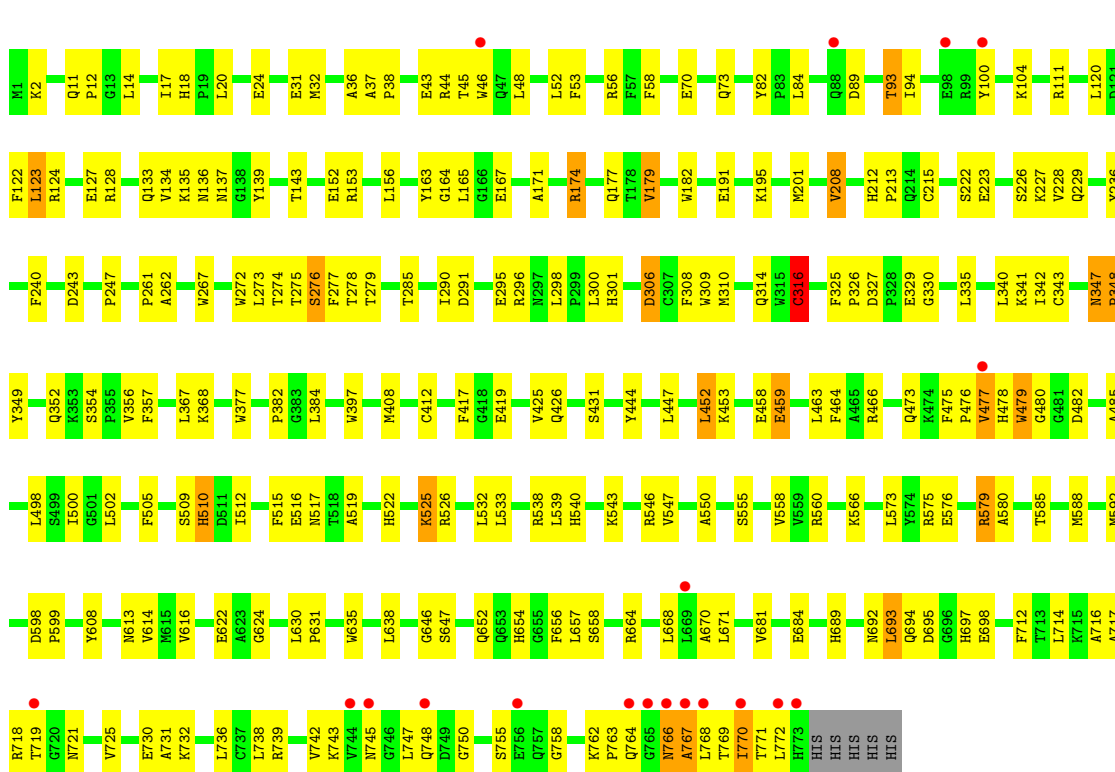
Chain B:





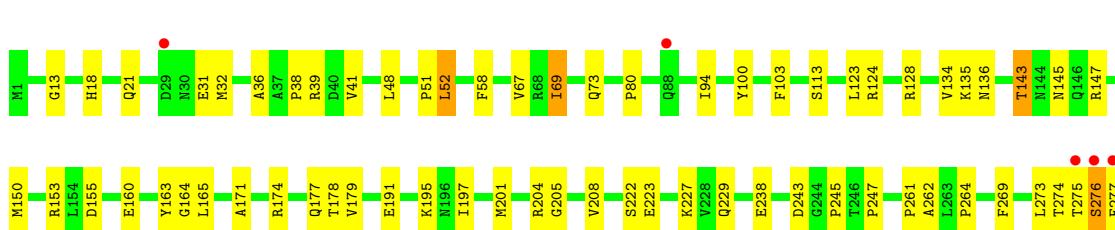
• Molecule 1: Putative family 31 glucosidase yicI

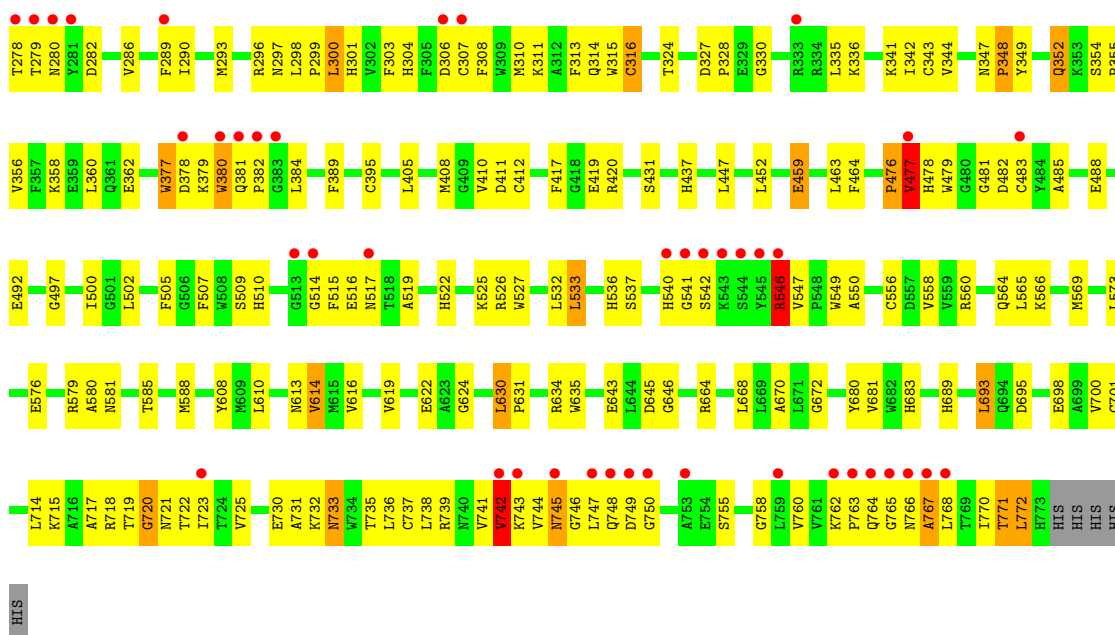
Chain C:

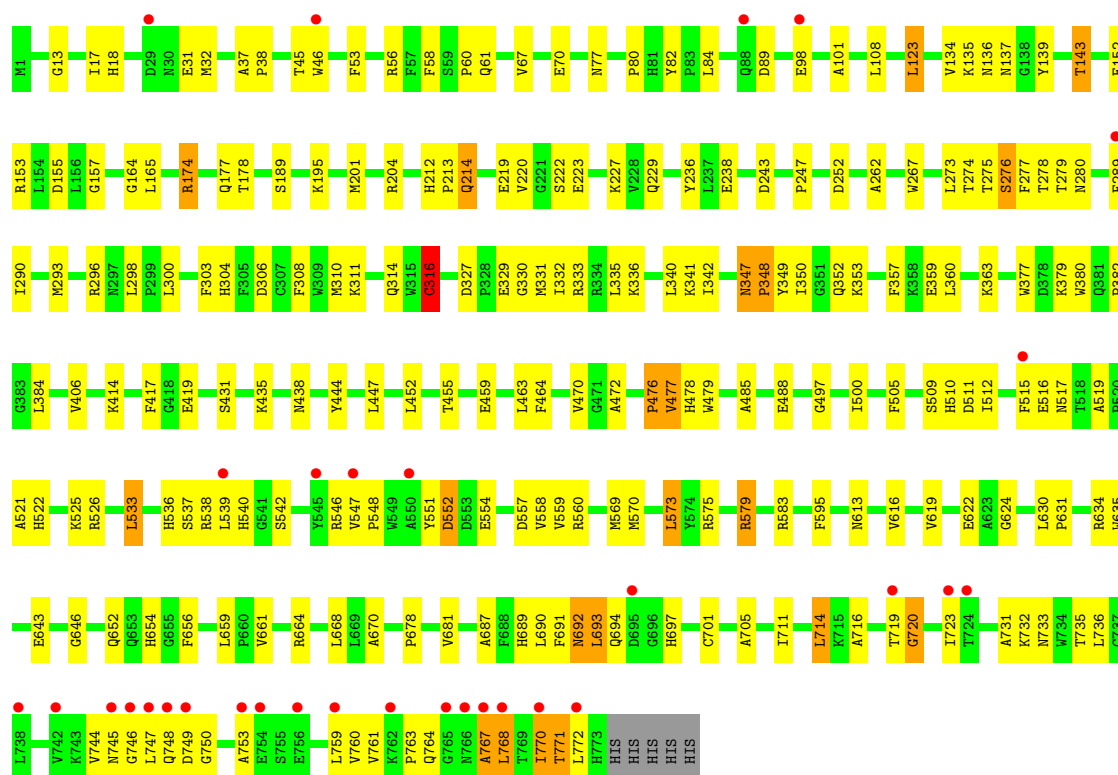


• Molecule 1: Putative family 31 glucosidase yicI

Chain D:







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 0.232 , 0.230	Depositor DCC
R_{free} test set	15006 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 296995 reflections	Xtriage
F_o, F_c correlation	0.93	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	7	2	0
3	B	10	0	7	1	0
3	C	10	0	7	2	0
3	E	10	0	7	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	35692	1212	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (1212) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:274:THR:HG22	1:A:276:SER:H	1.14	1.11

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Atom-1	Atom-2	Distance(Å)	Clash(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:280:ASN:HA	1:E:44:ARG:HH21	1.37	0.87
1:D:547:VAL:HG23	1:D:550:ALA:HB2	1.55	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
1:A:368:LYS:O	1:A:425:VAL:HG23	1.79	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:329:GLU:HG3	1:C:408:MET:HG3	1.62	0.81
1:A:463:LEU:O	1:A:477:VAL:HG22	1.81	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:F:274:THR:HG21	1:F:540:HIS:ND1	1.97	0.79
1:B:136:ASN:HD21	1:B:227:LYS:HE3	1.47	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:D:725:VAL:HB	1:D:768:LEU:HD12	1.67	0.76
1:C:201:MET:HE1	1:C:247:PRO:HB3	1.66	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:D:540:HIS:C	1:D:546:ARG:HE	1.90	0.75
1:A:761:VAL:HG11	1:A:768:LEU:HD21	1.69	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:F:347:ASN:HD22	1:F:347:ASN:C	1.91	0.74
1:E:673:ASN:HD22	1:E:685:GLY:HA3	1.52	0.74
1:B:157:GLY:HA3	1:B:204:ARG:NH2	2.01	0.74
1:B:332:ILE:HD12	1:B:333:ARG:N	2.01	0.74
1:A:635:TRP:CH2	1:A:664:ARG:HG2	2.23	0.74
1:C:579:ARG:NH1	1:C:579:ARG:HB2	2.00	0.74
1:E:694:GLN:HB2	1:E:697:HIS:CD2	2.19	0.73
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
1:B:689:HIS:ND1	1:B:739:ARG:NH1	2.36	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:755:SER:HB3	1:C:758:GLY:O	1.88	0.73
1:C:352:GLN:NE2	1:D:73:GLN:HG3	2.04	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: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:C:731:ALA:O	1:C:732:LYS:HD2	1.90	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:D:377:TRP:HH2	1:D:420:ARG:HD3	1.54	0.71
1:C:174:ARG:O	1:C:177:GLN:HG2	1.90	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:F:635:TRP:CH2	1:F:664:ARG:HG2	2.27	0.70
1:D:522:HIS:CG	1:D:622:GLU:HG3	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:367:LEU:HD11	1:C:425:VAL:HG21	1.74	0.69
1:C:725:VAL:HB	1:C:768:LEU:HB3	1.75	0.69
1:F:382:PRO:HG2	5:F:3046:HOH:O	1.91	0.69
1:A:742:VAL:HG23	1:A:743:LYS:H	1.57	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
1:B:742:VAL:HG23	1:B:743:LYS:H	1.58	0.68
1:A:352:GLN:NE2	1:B:73:GLN:HG3	2.07	0.68
1:F:311:LYS:HE3	1:F:314:GLN:OE1	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:E:673:ASN:ND2	1:E:685:GLY:HA3	2.08	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:F:347:ASN:ND2	1:F:349:TYR:H	1.93	0.67
1:C:133:GLN:HB2	1:C:136:ASN:HD22	1.59	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: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:174:ARG:O	1:B:177:GLN:HG2	1.95	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:C:512:ILE:HB	1:C:539:LEU:HD23	1.77	0.65
1:A:165:LEU:HD12	1:A:174:ARG:HG2	1.78	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:A:347:ASN:HD22	1:A:347:ASN:C	1.99	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:E:377:TRP:CZ3	1:E:379:LYS:HD2	2.31	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:B:123:LEU:N	1:B:123:LEU:HD22	2.11	0.65
1:A:16:LEU:HD22	1:A:140:VAL:HG22	1.79	0.65
1:D:485:ALA:CB	1:D:519:ALA:HB2	2.23	0.65
1:C:692:ASN:H	1:C:692:ASN:HD22	1.43	0.65
1:E:329:GLU:O	1:E:333:ARG:HG2	1.97	0.65
1:D:540:HIS:CG	1:D:541:GLY:H	2.14	0.65
1:C:638:LEU:O	1:C:739:ARG:NH2	2.30	0.65
1:E:417:PHE:HA	1:E:419:GLU:OE2	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:E:476:PRO:O	1:E:477:VAL:CG1	2.45	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:E:565:LEU:HG	1:E:569:MET:HE2	1.78	0.64
1:D:417:PHE:HA	1:D:419:GLU:OE2	1.97	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:D:565:LEU:HG	1:D:569:MET:HE2	1.80	0.64
1:B:681:VAL:O	1:B:681:VAL:HG13	1.97	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:F:274:THR:HG23	1:F:304:HIS:HD2	1.63	0.63
1:C:692:ASN:N	1:C:692:ASN:HD22	1.96	0.63
1:C:31:GLU:OE1	1:C:56:ARG:HD3	1.99	0.63
1:C:367:LEU:HG	1:C:425:VAL:HG21	1.81	0.63
1:C:153:ARG:HG2	1:C:229:GLN:HB2	1.80	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:F:476:PRO:O	1:F:477:VAL:HG12	1.99	0.63
1:B:476:PRO:O	1:B:477:VAL:HG12	1.99	0.63
1:B:459:GLU:CD	1:B:459:GLU:H	2.00	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: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:D:565:LEU:HG	1:D:569:MET:CE	2.29	0.62
1:D:532:LEU:O	1:D:566:LYS:HD2	2.00	0.62
1:B:347:ASN:C	1:B:347:ASN:HD22	2.03	0.62
1:D:540:HIS:CG	1:D:541:GLY:N	2.67	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:693:LEU:HD11	1:C:716:ALA:O	2.00	0.61
1:C:382:PRO:HG2	5:C:3013:HOH: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:579:ARG:CG	1:C:579:ARG:HH11	2.13	0.61
1:C:425:VAL:CG2	1:C:426:GLN:H	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:C:275:THR:O	1:C:276:SER:HB2	2.01	0.61
1:B:307:CYS:HB3	1:B:315:TRP:CZ2	2.36	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:F:195:LYS:HE2	1:F:478:HIS:HB3	1.83	0.61
1:B:766:ASN:O	1:B:767:ALA:HB3	2.00	0.61
1:D:379:LYS:O	1:D:380:TRP:HB3	2.01	0.61
1:C:689:HIS:ND1	1:C:739:ARG:NH1	2.48	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:F:275:THR:O	1:F:276:SER:HB2	2.01	0.61
1:C:300:LEU:HD12	1:C:340:LEU:CD2	2.30	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:D:766:ASN:C	1:D:768:LEU:N	2.53	0.60
1:A:2:LYS:HE3	1:D:191:GLU:OE2	2.01	0.60
1:A:414:LYS:HZ2	1:A:538:ARG:HH12	1.49	0.60
1:E:273:LEU:HB2	1:E:300:LEU:HD21	1.82	0.60
1:F:579:ARG:HG3	1:F:579:ARG:HH11	1.65	0.60
1:E:21:GLN:NE2	1:E:42:ARG:HG3	2.17	0.60
1:C:417:PHE:HA	1:C:419:GLU:OE2	2.02	0.60
1:E:772:LEU:HD22	1:E:772:LEU:H	1.65	0.60
1:E:565:LEU:HG	1:E:569:MET:HE1	1.84	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:F:296:ARG:O	1:F:560:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:540:HIS:C	1:F:546:ARG:HG3	2.22	0.60
1:A:290:ILE:CD1	1:A:335:LEU:HD22	2.32	0.60
1:E:274:THR:HG21	1:E:540:HIS:CE1	2.36	0.59
1:A:368:LYS:O	1:A:425:VAL:CG2	2.50	0.59
1:D:731:ALA:O	1:D:732:LYS:HD2	2.02	0.59
1:B:547:VAL:HG23	1:B:550:ALA:HB2	1.82	0.59
1:F:347:ASN:C	1:F:347:ASN:ND2	2.55	0.59
1:D:463:LEU:O	1:D:477:VAL:HG13	2.01	0.59
1:F:750:GLY:HA2	1:F:764:GLN:HG2	1.84	0.59
1:B:311:LYS:HE3	1:B:314:GLN:OE1	2.02	0.59
1:C:300:LEU:HD12	1:C:340:LEU:HD22	1.83	0.59
1:D:546:ARG:CA	1:D:546:ARG:HH11	2.15	0.59
1:C:684:GLU:HG2	1:C:732:LYS:HB2	1.85	0.59
1:C:463:LEU:O	1:C:477:VAL:HB	2.02	0.59
1:F:681:VAL:HG12	2:F:3005:SO4:O3	2.02	0.59
1:E:31:GLU:OE1	1:E:56:ARG:HD3	2.02	0.59
1:B:671:LEU:HD12	1:B:671:LEU:N	2.18	0.59
1:A:163:TYR:HB3	1:A:502:LEU:HD13	1.85	0.59
1:B:123:LEU:HA	1:B:127:GLU:O	2.03	0.59
1:A:342:ILE:HD12	1:A:342:ILE:N	2.18	0.59
1:F:352:GLN:HA	1:F:357:PHE:CD2	2.37	0.59
1:B:748:GLN:CG	1:B:769:THR:HB	2.32	0.59
1:B:31:GLU:OE1	1:B:56:ARG:HD3	2.02	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:E:635:TRP:CH2	1:E:664:ARG:HG2	2.38	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: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
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:F:300:LEU:HD12	1:F:340:LEU:CD2	2.34	0.58
1:D:747:LEU:HD22	1:D:750:GLY:O	2.04	0.58
1:D:352:GLN:OE1	1:E:73:GLN:N	2.33	0.58
1:F:310:MET:SD	1:F:316:CYS:HA	2.44	0.58
1:E:536:HIS:HA	5:E:3025:HOH:O	2.04	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:214:GLN:HE22	1:E:232:VAL:CG2	2.17	0.58
1:F:747:LEU:HD22	1:F:750:GLY:O	2.04	0.58
1:E:516:GLU:O	1:E:517:ASN:HB2	2.03	0.58
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:A:134:VAL:O	1:A:135:LYS:HB2	2.04	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:348:PRO:O	1:B:387:TYR:HD1	1.87	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:E:547:VAL:HG23	1:E:550:ALA:HB2	1.86	0.57
1:F:719:THR:HG23	1:F:720:GLY:N	2.20	0.57
1:D:695:ASP:HA	1:D:718:ARG:HD3	1.86	0.57
1:F:447:LEU:C	1:F:447:LEU:HD23	2.24	0.57
1:F:548:PRO:HG3	1:F:559:VAL:HG21	1.86	0.57
1:C:165:LEU:HD13	1:C:179:VAL:HG21	1.87	0.57
1:C:123:LEU:HD22	1:C:123:LEU:N	2.20	0.57
1:E:35:TYR:HB3	1:E:52:LEU:HD11	1.87	0.57
1:B:28:GLN:NE2	1:B:33:VAL:HG21	2.19	0.57
1:A:580:ALA:HA	1:A:585:THR:O	2.04	0.57
1:D:298:LEU:CD2	1:D:560:ARG:HB2	2.35	0.57
1:A:123:LEU:HD13	1:A:128:ARG:HA	1.85	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: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:A:742:VAL:HG23	1:A:743:LYS:N	2.21	0.56
1:C:384:LEU:HD23	1:C:384:LEU:C	2.25	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:E:522:HIS:CG	1:E:622:GLU:HG3	2.40	0.56
1:A:377:TRP:CZ3	1:A:379:LYS:HD2	2.41	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:174:ARG:HB3	1:E:220:VAL:HG11	1.87	0.56
1:C:134:VAL:O	1:C:135:LYS:HB2	2.06	0.56
1:E:539:LEU:HB3	1:E:546:ARG:HB3	1.88	0.56
1:C:296:ARG:O	1:C:560:ARG:NH1	2.39	0.56
1:A:275:THR:O	1:A:276:SER:HB2	2.04	0.56
1:F:485:ALA:HB1	1:F:519:ALA:CB	2.25	0.56
1:C:516:GLU:O	1:C:517:ASN:HB2	2.06	0.56
1:B:350:ILE:HD13	1:B:360:LEU:HD12	1.87	0.56
1:F:137:ASN:HB3	1:F:152:GLU:OE1	2.05	0.56
1:E:311:LYS:HE3	1:E:314:GLN:OE1	2.06	0.56
1:C:290:ILE:CD1	1:C:335:LEU:HD22	2.36	0.56
1:B:476:PRO:O	1:B:477:VAL:CG1	2.53	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:B:164:GLY:O	1:B:165:LEU:HB2	2.06	0.55
1:A:48:LEU:HD12	1:A:49:ASP:HB2	1.88	0.55
1:F:476:PRO:O	1:F:477:VAL:CG1	2.54	0.55
1:F:165:LEU:HD12	1:F:174:ARG:HG2	1.88	0.55
1:C:18:HIS:O	1:C:38:PRO:HA	2.06	0.55
1:A:692:ASN:HD22	1:A:692:ASN:H	1.52	0.55
1:F:746:GLY:N	1:F:771:THR:HG23	2.21	0.55
1:C:525:LYS:CG	1:C:558:VAL:HG21	2.33	0.55
1:C:124:ARG:NH2	1:C:243:ASP:OD1	2.38	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:482:ASP:HB3	1:D:516:GLU:OE1	2.07	0.55
1:D:18:HIS:O	1:D:38:PRO:HA	2.07	0.55
1:E:44:ARG:HG2	1:E:47:GLN:HE22	1.71	0.55
1:A:770:ILE:HD12	1:A:770:ILE:C	2.27	0.55
1:A:43:GLU:HB2	1:A:46:TRP:HD1	1.71	0.55
1:C:459:GLU:H	1:C:459:GLU:CD	2.02	0.55
1:E:742:VAL:HG23	1:E:743:LYS:N	2.22	0.55
1:B:762:LYS:HD2	1:B:763:PRO:HD2	1.88	0.55
1:E:195:LYS:HE2	1:E:478:HIS:HB3	1.87	0.55
1:D:672:GLY:HA3	1:D:680:TYR:OH	2.07	0.55
1:B:500:ILE:HG12	1:B:505:PHE:HB2	1.88	0.55
1:D:735:THR:CG2	1:D:736:LEU:N	2.70	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:C:348:PRO:HG2	1:C:349:TYR:CE1	2.42	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:285:THR:O	1:B:288:SER:HB3	2.07	0.55
1:A:447:LEU:C	1:A:447:LEU:HD23	2.27	0.55
1:F:274:THR:HG21	1:F:540:HIS:CE1	2.42	0.54
1:B:730:GLU:HG3	1:B:732:LYS:NZ	2.22	0.54
1:B:722:THR:HG23	1:B:769:THR:HG23	1.89	0.54
1:E:718:ARG:HB2	1:E:723:ILE:HG22	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:B:648:ARG:HD3	5:C:3115:HOH:O	2.06	0.54
1:C:347:ASN:ND2	1:C:347:ASN:C	2.61	0.54
1:E:479:TRP:CZ2	3:E:804:XYF:H2	2.42	0.54
1:F:744:VAL:HG22	1:F:745:ASN:N	2.22	0.54
1:C:261:PRO:HA	1:C:473:GLN:O	2.08	0.54
1:E:500:ILE:HG12	1:E:505:PHE:HB2	1.89	0.54
1:E:133:GLN:HB2	1:E:136:ASN:HD22	1.72	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:B:382:PRO:HG2	5:B:3011:HOH:O	2.08	0.54
1:F:331:MET:O	1:F:335:LEU:HG	2.08	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: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:F:575:ARG:NH2	1:F:579:ARG:HH12	2.05	0.54
1:F:526:ARG:HD2	1:F:619:VAL:HB	1.90	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:C:575:ARG:NH1	1:C:579:ARG:HH12	2.05	0.54
1:E:522:HIS:CE1	1:E:523:VAL:HG23	2.42	0.54
1:D:735:THR:CG2	1:D:760:VAL:HG13	2.38	0.54
1:C:277:PHE:CD2	1:C:278:THR:HG23	2.42	0.54
1:B:201:MET:CE	1:B:247:PRO:HB3	2.38	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: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:B:479:TRP:HZ2	3:B:802:XYF:H2	1.73	0.54
1:C:291:ASP:O	1:C:295:GLU:HG3	2.08	0.54
1:F:336:LYS:HG2	1:F:342:ILE:CD1	2.37	0.54
1:F:17:ILE:HG12	1:F:139:TYR:HB3	1.90	0.54
1:A:479:TRP:HZ2	3:A:801:XYF:H2	1.73	0.54
1:F:384:LEU:HD23	1:F:384:LEU:C	2.28	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:352:GLN:HA	1:E:357:PHE:CD2	2.43	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:D:483:CYS:SG	1:D:514:GLY:HA2	2.48	0.53
1:C:327:ASP:OD2	1:C:330:GLY:HA3	2.06	0.53
1:A:766:ASN:O	1:A:767:ALA:HB2	2.08	0.53
1:F:735:THR:HG22	1:F:736:LEU:N	2.23	0.53
1:D:772:LEU:H	1:D:772:LEU:HD22	1.72	0.53
1:E:735:THR:CG2	1:E:736:LEU:N	2.72	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:A:311:LYS:HE3	1:A:314:GLN:OE1	2.08	0.53
1:F:497:GLY:O	1:F:500:ILE:HG22	2.09	0.53
1:F:267:TRP:CE3	1:F:341:LYS:HG3	2.44	0.53
1:B:310:MET:SD	1:B:316:CYS:HA	2.49	0.53
1:F:668:LEU:O	1:F:701:CYS:HB2	2.09	0.53
1:E:745:ASN:HB3	1:E:771:THR:O	2.09	0.53
1:A:136:ASN:HB3	1:A:153:ARG:HB2	1.90	0.53
1:F:70:GLU:HB3	1:F:236:TYR:HB2	1.90	0.53
1:C:447:LEU:C	1:C:447:LEU:HD23	2.28	0.53
1:B:315:TRP:HB2	1:B:381:GLN:OE1	2.09	0.53
1:B:352:GLN:HA	1:B:357:PHE:CD2	2.43	0.53
1:A:17:ILE:O	1:A:17:ILE:HG13	2.07	0.53
1:B:668:LEU:HD13	1:B:690:LEU:HD13	1.91	0.53
1:E:333:ARG:HH11	1:E:336:LYS:HE3	1.73	0.53
1:D:282:ASP:O	1:D:286:VAL:HG23	2.09	0.53
1:E:552:ASP:OD1	1:E:555:SER:N	2.38	0.53
1:C:694:GLN:HB2	1:C:697:HIS:CD2	2.44	0.53
1:F:472:ALA:HB1	5:F:3084:HOH:O	2.08	0.53
1:D:310:MET:SD	1:D:316:CYS:HA	2.48	0.53
1:F:277:PHE:CD2	1:F:278:THR:HG23	2.44	0.53
1:D:547:VAL:CG2	1:D:550:ALA:HB2	2.34	0.53
1:B:16:LEU:HD22	1:B:140:VAL:HG22	1.90	0.53
1:E:749:ASP:C	1:E:764:GLN:HE22	2.13	0.53
1:D:509:SER:HB3	1:D:536:HIS:HB2	1.91	0.53
1:C:742:VAL:HG23	1:C:743:LYS:N	2.24	0.53
1:F:153:ARG:HG2	1:F:229:GLN:HB2	1.91	0.53
1:F:274:THR:HG22	1:F:275:THR:N	2.25	0.52
1:E:681:VAL:HG13	1:E:681:VAL:O	2.09	0.52
1:A:343:CYS:HB2	1:A:412:CYS:SG	2.49	0.52
1:B:262:ALA:HB3	1:B:476:PRO:HG3	1.90	0.52
1:E:744:VAL:HG21	1:E:770:ILE:CG2	2.39	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:742:VAL:HG23	1:E:743:LYS:H	1.74	0.52
1:B:61:GLN:NE2	1:B:87:LEU:HG	2.23	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: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:453:LYS:HD2	1:C:458:GLU:OE1	2.09	0.52
1:B:298:LEU:CD2	1:B:560:ARG:HB2	2.39	0.52
1:D:766:ASN:O	1:D:768:LEU:N	2.42	0.52
1:F:174:ARG:HB3	1:F:220:VAL:HG11	1.92	0.52
1:F:719:THR:HG23	1:F:720:GLY:H	1.73	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:F:327:ASP:OD2	1:F:330:GLY:HA3	2.08	0.52
1:E:267:TRP:CE3	1:E:341:LYS:HG3	2.44	0.52
1:E:43:GLU:C	1:E:45:THR:H	2.13	0.52
1:C:201:MET:CE	1:C:247:PRO:HB3	2.38	0.52
1:B:479:TRP:HA	1:B:509:SER:O	2.10	0.52
1:E:468:ALA:HB1	1:E:472:ALA:HB3	1.91	0.52
1:A:588:MET:HE3	5:A:3065:HOH:O	2.08	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:F:557:ASP:OD1	1:F:560:ARG:NH2	2.43	0.52
1:B:384:LEU:HD23	1:B:384:LEU:C	2.31	0.52
1:A:80:PRO:HD3	1:A:431:SER:HB3	1.91	0.52
1:A:719:THR:HG23	1:A:720:GLY:H	1.75	0.52
1:E:479:TRP:CH2	3:E:804:XYF:H2	2.45	0.52
1:F:290:ILE:CD1	1:F:335:LEU:HD22	2.39	0.52
1:D:719:THR:HG22	1:D:722:THR:HB	1.92	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:D:681:VAL:HG13	1:D:681:VAL:O	2.09	0.52
1:D:80:PRO:HD3	1:D:431:SER:HB3	1.91	0.52
1:F:516:GLU:O	1:F:517:ASN:HB2	2.09	0.52
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: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:A:347:ASN:HA	1:A:444:TYR:OH	2.11	0.51
1:E:377:TRP:HE1	1:E:384:LEU:HD22	1.75	0.51
1:C:18:HIS:HB2	1:C:20:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:31:GLU:HG2	1:D:58:PHE:HB3	1.92	0.51
1:B:638:LEU:O	1:B:739:ARG:NH2	2.44	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:C:306:ASP:O	1:C:309:TRP:HD1	1.94	0.51
1:A:31:GLU:OE1	1:A:56:ARG:HD3	2.10	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:D:689:HIS:ND1	1:D:739:ARG:NE	2.53	0.51
1:A:18:HIS:O	1:A:38:PRO:HA	2.10	0.51
1:E:306:ASP:O	1:E:309:TRP:HD1	1.93	0.51
1:B:744:VAL:HG23	1:B:772:LEU:HA	1.93	0.51
1:B:31:GLU:HG2	1:B:58:PHE:HB3	1.91	0.51
1:A:122:PHE:C	1:A:123:LEU:HD22	2.31	0.51
1:B:17:ILE:HG13	1:B:53:PHE:HZ	1.75	0.51
1:A:630:LEU:O	1:A:647:SER:N	2.43	0.51
1:A:748:GLN:HB2	1:A:769:THR:HG22	1.91	0.51
1:A:635:TRP:CZ3	1:A:664:ARG:HG2	2.46	0.51
1:E:497:GLY:O	1:E:500:ILE:HG22	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:F:134:VAL:O	1:F:135:LYS:HB2	2.11	0.51
1:E:150:MET:HB3	1:E:237:LEU:HB2	1.92	0.51
1:F:276:SER:HB2	1:F:279:THR:OG1	2.10	0.51
1:D:547:VAL:HG23	1:D:550:ALA:CB	2.33	0.51
1:B:274:THR:HG23	1:B:304:HIS:HD2	1.76	0.51
1:E:20:LEU:HD12	1:E:38:PRO:O	2.11	0.51
1:C:515:PHE:CD1	1:C:516:GLU:HG2	2.46	0.51
1:F:214:GLN:HG3	1:F:435:LYS:HG2	1.93	0.51
1:E:134:VAL:O	1:E:135:LYS:HB2	2.11	0.51
1:A:310:MET:SD	1:A:316:CYS:HA	2.51	0.51
1:D:293:MET:CE	1:D:300:LEU:HD23	2.41	0.50
1:A:723:ILE:O	1:A:723:ILE:HG13	2.11	0.50
1:F:767:ALA:O	1:F:768:LEU:C	2.49	0.50
1:E:343:CYS:HB2	1:E:412:CYS:SG	2.52	0.50
1:B:274:THR:CG2	1:B:275:THR:N	2.75	0.50
1:E:287:ASN:HD21	1:E:334:ARG:HH21	1.59	0.50
1:A:201:MET:HE1	1:A:247:PRO:CA	2.39	0.50
1:E:293:MET:HE2	1:E:300:LEU:HD23	1.94	0.50
1:D:165:LEU:HA	1:D:197:ILE:O	2.11	0.50
1:E:767:ALA:O	1:E:769:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:380:TRP:H	1:E:49:ASP:HA	1.75	0.50
1:D:476:PRO:O	1:D:477:VAL:CG1	2.60	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:670:ALA:HB2	1:D:701:CYS:SG	2.51	0.50
1:A:274:THR:CG2	1:A:275:THR:N	2.74	0.50
1:D:630:LEU:HG	1:D:635:TRP:CD1	2.46	0.50
1:D:201:MET:CE	1:D:247:PRO:HB3	2.42	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:B:723:ILE:O	1:B:723:ILE:HG13	2.10	0.50
1:B:671:LEU:HD13	1:B:689:HIS:HD2	1.77	0.50
1:D:378:ASP:HA	1:D:381:GLN:O	2.11	0.50
1:A:735:THR:CG2	1:A:760:VAL:HG13	2.41	0.50
1:B:332:ILE:HG12	1:B:408:MET:O	2.12	0.50
1:D:32:MET:HE1	1:D:94:ILE:HG23	1.91	0.50
1:C:133:GLN:HB2	1:C:136:ASN:ND2	2.26	0.50
1:B:379:LYS:O	1:B:380:TRP:HB3	2.11	0.50
1:A:380:TRP:CD1	1:A:381:GLN:HG2	2.47	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: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:A:273:LEU:HD12	1:A:303:PHE:CE1	2.47	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:A:61:GLN:HB2	1:A:64:ILE:HD12	1.94	0.50
1:C:654:HIS:ND1	1:C:658:SER:OG	2.35	0.50
1:E:214:GLN:NE2	1:E:232:VAL:CG2	2.75	0.50
1:F:692:ASN:N	1:F:692:ASN:HD22	2.06	0.50
1:F:554:GLU:O	1:F:558:VAL:HG23	2.12	0.50
1:D:500:ILE:HG12	1:D:505:PHE:HB2	1.94	0.50
1:B:45:THR:HG23	1:B:46:TRP:CD1	2.47	0.50
1:A:16:LEU:CD2	1:A:140:VAL:HG22	2.40	0.49
1:E:38:PRO:HG2	1:E:51:PRO:HB2	1.94	0.49
1:E:293:MET:CE	1:E:300:LEU:HD23	2.42	0.49
1:D:693:LEU:HD13	1:D:718:ARG:HB2	1.94	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:546:ARG:N	1:D:546:ARG:HH11	2.09	0.49
1:C:747:LEU:HD22	1:C:750:GLY:O	2.12	0.49
1:F:17:ILE:CG1	1:F:139:TYR:HB3	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:588:MET:HE3	5:D:3075:HOH:O	2.12	0.49
1:E:489:SER:O	1:E:492:GLU:HG2	2.12	0.49
1:D:733:ASN:OD1	1:D:733:ASN:O	2.29	0.49
1:D:770:ILE:N	1:D:770:ILE:HD12	2.28	0.49
1:C:347:ASN:HA	1:C:444:TYR:OH	2.12	0.49
1:F:579:ARG:NH1	1:F:579:ARG:HG3	2.27	0.49
1:A:182:TRP:CE3	1:A:215:CYS:HB2	2.48	0.49
1:D:160:GLU:HG3	1:D:204:ARG:HG2	1.94	0.49
1:C:163:TYR:HB3	1:C:502:LEU:HD13	1.94	0.49
1:C:70:GLU:HG2	5:C:3100:HOH:O	2.11	0.49
1:C:274:THR:HG21	1:C:540:HIS:CG	2.48	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:298:LEU:HD23	1:C:560:ARG:HG3	1.93	0.49
1:F:219:GLU:HB2	1:F:229:GLN:HB3	1.93	0.49
1:E:748:GLN:HB2	1:E:769:THR:OG1	2.13	0.49
1:D:749:ASP:OD2	1:D:767:ALA:HB3	2.12	0.49
1:D:738:LEU:HB2	1:D:741:VAL:HB	1.94	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:E:305:PHE:HB2	1:E:344:VAL:HG12	1.95	0.49
1:C:479:TRP:CZ2	3:C:803:XYF:H2	2.48	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:F:414:LYS:NZ	1:F:538:ARG:HH22	2.10	0.49
1:E:763:PRO:O	1:E:764:GLN:HB3	2.12	0.49
1:E:548:PRO:HG3	1:E:559:VAL:HG21	1.95	0.49
1:F:18:HIS:O	1:F:38:PRO:HA	2.13	0.49
1:B:447:LEU:C	1:B:447:LEU:HD23	2.33	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:E:772:LEU:N	1:E:772:LEU:HD22	2.28	0.49
1:F:438:ASN:HB3	5:F:3119:HOH:O	2.12	0.49
1:A:576:GLU:HG3	1:A:611:GLY:HA3	1.93	0.49
1:B:273:LEU:HD12	1:B:303:PHE:HE1	1.78	0.49
1:B:152:GLU:HB3	1:B:230:PHE:CE1	2.48	0.49
1:E:747:LEU:HD22	1:E:750:GLY:O	2.13	0.49
1:E:124:ARG:NH2	1:E:243:ASP:OD1	2.46	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:D:698:GLU:OE1	1:D:715:LYS:HD3	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:134:VAL:HG22	1:F:135:LYS:HG3	1.95	0.49
1:A:417:PHE:HA	1:A:419:GLU:OE2	2.12	0.49
1:C:670:ALA:C	1:C:671:LEU:HD12	2.33	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:A:453:LYS:HG3	1:A:458:GLU:HG3	1.93	0.49
1:F:82:TYR:HB3	1:F:84:LEU:HD13	1.95	0.49
1:F:719:THR:HG22	5:F:3140:HOH:O	2.13	0.48
1:A:58:PHE:N	1:A:58:PHE:CD1	2.81	0.48
1:C:652:GLN:NE2	1:C:654:HIS:NE2	2.60	0.48
1:C:356:VAL:HG11	1:C:397:TRP:CH2	2.48	0.48
1:D:145:ASN:OD1	1:D:147:ARG:HB2	2.13	0.48
1:B:204:ARG:HD2	1:B:206:TYR:HE2	1.79	0.48
1:E:723:ILE:CG1	1:E:770:ILE:HB	2.41	0.48
1:C:82:TYR:HB2	1:C:84:LEU:CD2	2.42	0.48
1:A:498:LEU:HD21	1:A:608:TYR:HB3	1.95	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:A:749:ASP:HB3	1:A:764:GLN:O	2.13	0.48
1:D:723:ILE:CG1	1:D:770:ILE:HB	2.43	0.48
1:B:16:LEU:CD2	1:B:140:VAL:HG22	2.43	0.48
1:E:277:PHE:CD2	1:E:278:THR:HG23	2.48	0.48
1:E:201:MET:CE	1:E:247:PRO:HA	2.43	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:B:347:ASN:HA	1:B:444:TYR:OH	2.14	0.48
1:F:336:LYS:HG2	1:F:342:ILE:HD13	1.94	0.48
1:E:634:ARG:NH2	1:E:634:ARG:HG3	2.28	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:F:280:ASN:HB3	5:F:3086:HOH:O	2.13	0.48
1:C:692:ASN:ND2	1:C:692:ASN:N	2.61	0.48
1:D:719:THR:CG2	1:D:722:THR:HB	2.44	0.48
1:F:522:HIS:CB	1:F:622:GLU:HG3	2.44	0.48
1:C:500:ILE:HG12	1:C:505:PHE:HB2	1.95	0.48
1:E:208:VAL:HA	1:E:240:PHE:O	2.13	0.48
1:D:515:PHE:CD1	1:D:542:SER:HB2	2.49	0.48
1:D:315:TRP:CE3	1:D:381:GLN:NE2	2.82	0.48
1:D:274:THR:OG1	1:D:304:HIS:HB3	2.14	0.48
1:B:332:ILE:HD12	1:B:332:ILE:C	2.34	0.48
1:E:300:LEU:HD13	1:E:301:HIS:N	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:136:ASN:HB3	1:F:153:ARG:HB2	1.96	0.48
1:E:282:ASP:HB3	1:E:324:THR:HG23	1.94	0.48
1:D:580:ALA:HA	1:D:585:THR:O	2.14	0.48
1:C:11:GLN:HB2	1:C:14:LEU:HD12	1.96	0.48
1:B:296:ARG:HD3	1:B:556:CYS:SG	2.53	0.48
1:A:405:LEU:O	1:A:408:MET:HB3	2.14	0.48
1:B:672:GLY:HA3	1:B:680:TYR:OH	2.13	0.48
1:E:274:THR:CG2	1:E:275:THR:N	2.77	0.48
1:F:515:PHE:CD1	1:F:542:SER:HB2	2.49	0.48
1:C:540:HIS:C	1:C:546:ARG:HG3	2.34	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:A:121:ASP:OD1	1:A:128:ARG:HD2	2.14	0.48
1:F:332:ILE:O	1:F:336:LYS:HG3	2.13	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:F:333:ARG:HH11	1:F:333:ARG:HG2	1.78	0.48
1:B:670:ALA:HB2	1:B:701:CYS:SG	2.54	0.48
1:F:277:PHE:HB3	1:F:542:SER:O	2.14	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:A:31:GLU:HG2	1:A:58:PHE:HB3	1.94	0.48
1:C:272:TRP:CB	1:C:538:ARG:HG3	2.44	0.48
1:C:272:TRP:HB2	1:C:538:ARG:HG3	1.94	0.48
1:F:262:ALA:HB3	1:F:476:PRO:HG3	1.95	0.48
1:E:100:TYR:CD2	1:E:113:SER:HA	2.49	0.48
1:D:698:GLU:HG3	1:D:717:ALA:HB2	1.95	0.48
1:C:579:ARG:NH1	1:C:579:ARG:CG	2.76	0.47
1:B:693:LEU:HD21	1:B:697:HIS:O	2.14	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:B:521:ALA:O	1:B:525:LYS:HD3	2.13	0.47
1:F:290:ILE:HD11	1:F:335:LEU:HD22	1.96	0.47
1:E:588:MET:HG3	1:E:608:TYR:CD1	2.48	0.47
1:C:772:LEU:N	1:C:772:LEU:HD22	2.29	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:B:476:PRO:C	1:B:477:VAL:HG12	2.34	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:E:43:GLU:HB3	1:E:45:THR:HG22	1.96	0.47
1:B:753:ALA:O	1:B:759:LEU:HD12	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:133:GLN:HB2	1:E:136:ASN:ND2	2.29	0.47
1:C:274:THR:HG23	1:C:276:SER:H	1.79	0.47
1:F:17:ILE:HG13	1:F:53:PHE:HZ	1.80	0.47
1:E:731:ALA:O	1:E:732:LYS:HD2	2.15	0.47
1:F:515:PHE:HE2	1:F:540:HIS:HE2	1.63	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:D:746:GLY:N	1:D:771:THR:HG23	2.30	0.47
1:B:277:PHE:HB3	1:B:542:SER:O	2.15	0.47
1:C:20:LEU:HD22	1:C:134:VAL:HG22	1.97	0.47
1:A:692:ASN:HD22	1:A:692:ASN:N	2.10	0.47
1:A:479:TRP:CZ2	3:A:801:XYF:H2	2.48	0.47
1:F:735:THR:CG2	1:F:760:VAL:HG13	2.45	0.47
1:E:298:LEU:HD13	1:E:548:PRO:HG2	1.96	0.47
1:A:261:PRO:HA	1:A:473:GLN:O	2.14	0.47
1:D:405:LEU:O	1:D:408:MET:HB3	2.15	0.47
1:F:659:LEU:O	1:F:661:VAL:HG23	2.14	0.47
1:D:437:HIS:HB3	5:D:3049:HOH:O	2.13	0.47
1:A:201:MET:CE	1:A:247:PRO:HA	2.45	0.47
1:B:509:SER:HB2	1:B:536:HIS:HB2	1.97	0.47
1:A:512:ILE:HA	1:A:527:TRP:CD1	2.50	0.47
1:E:191:GLU:HB3	1:F:222:SER:O	2.14	0.47
1:B:274:THR:HG21	1:B:540:HIS:CE1	2.49	0.47
1:A:497:GLY:O	1:A:500:ILE:HG22	2.14	0.47
1:A:692:ASN:H	1:A:692:ASN:ND2	2.13	0.47
1:D:772:LEU:N	1:D:772:LEU:HD22	2.30	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:E:80:PRO:HD3	1:E:431:SER:HB3	1.96	0.47
1:E:290:ILE:HD12	1:E:335:LEU:HD22	1.96	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:C:747:LEU:HD23	1:C:748:GLN:N	2.29	0.46
1:B:64:ILE:HG12	1:B:242:ILE:HG23	1.97	0.46
1:C:510:HIS:CD2	1:C:510:HIS:N	2.82	0.46
1:F:687:ALA:O	1:F:689:HIS:HD2	1.98	0.46
1:D:634:ARG:HH21	1:D:634:ARG:HG3	1.80	0.46
1:A:749:ASP:C	1:A:764:GLN:HB2	2.36	0.46
1:D:560:ARG:O	1:D:564:GLN:HG3	2.16	0.46
1:A:123:LEU:HD22	1:A:123:LEU:N	2.31	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:296:ARG:HG3	1:E:296:ARG:HH11	1.80	0.46
1:B:364:GLY:HA2	5:B:3104:HOH:O	2.15	0.46
1:A:352:GLN:HA	1:A:357:PHE:CD2	2.50	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: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:B:44:ARG:HA	1:B:47:GLN:CG	2.42	0.46
1:A:761:VAL:CG1	1:A:768:LEU:HD21	2.43	0.46
1:F:735:THR:CG2	1:F:736:LEU:N	2.78	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:A:70:GLU:HG3	5:A:3171:HOH:O	2.16	0.46
1:F:747:LEU:HD23	1:F:748:GLN:N	2.31	0.46
1:C:17:ILE:O	1:C:17:ILE:HG13	2.14	0.46
1:F:275:THR:O	1:F:276:SER:CB	2.62	0.46
1:D:278:THR:CG2	1:E:45:THR:HA	2.45	0.46
1:B:525:LYS:O	1:B:528:CYS:HB2	2.16	0.46
1:B:341:LYS:O	1:B:342:ILE:HD12	2.15	0.46
1:A:273:LEU:C	1:A:273:LEU:HD13	2.36	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
1:A:693:LEU:HD22	1:A:718:ARG:HB3	1.97	0.46
1:A:290:ILE:HD13	1:A:340:LEU:CD1	2.46	0.46
1:E:41:VAL:C	1:E:43:GLU:H	2.18	0.46
1:D:738:LEU:CB	1:D:741:VAL:HB	2.46	0.46
1:F:525:LYS:HD3	1:F:656:PHE:CG	2.51	0.46
1:C:452:LEU:HA	1:C:452:LEU:HD12	1.76	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:E:287:ASN:ND2	1:E:334:ARG:HH21	2.14	0.45
1:C:84:LEU:N	1:C:84:LEU:HD22	2.31	0.45
1:C:167:GLU:OE2	1:C:195:LYS:NZ	2.43	0.45
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:F:569:MET:CB	1:F:573:LEU:HD22	2.46	0.45
1:E:248:LYS:HB2	2:E:3006:SO4:O4	2.16	0.45
1:C:262:ALA:HB3	1:C:476:PRO:HG3	1.97	0.45
1:B:717:ALA:O	1:B:723:ILE:HA	2.15	0.45
1:B:304:HIS:HA	1:B:343:CYS:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:48:LEU:HD12	1:E:49:ASP:OD2	2.16	0.45
1:D:269:PHE:O	1:D:566:LYS:HE2	2.15	0.45
1:F:289:PHE:CD1	1:F:547:VAL:HG11	2.51	0.45
1:E:129:ILE:HG22	1:E:204:ARG:NH1	2.30	0.45
1:A:719:THR:HG23	1:A:720:GLY:N	2.31	0.45
1:D:297:ASN:O	1:D:299:PRO:HD3	2.16	0.45
1:C:588:MET:HE3	5:C:3030:HOH:O	2.17	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: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:F:746:GLY:H	1:F:771:THR:HG23	1.82	0.45
1:E:136:ASN:HB3	1:E:153:ARG:HB2	1.98	0.45
1:F:500:ILE:HG12	1:F:505:PHE:HB2	1.98	0.45
1:D:719:THR:HG23	1:D:720:GLY:N	2.32	0.45
1:F:201:MET:CE	1:F:247:PRO:HB3	2.47	0.45
1:D:205:GLY:HA3	1:D:245:PRO:O	2.15	0.45
1:E:165:LEU:HD13	1:E:179:VAL:CG1	2.38	0.45
1:C:525:LYS:HD2	1:C:555:SER:HA	1.99	0.45
1:F:732:LYS:N	1:F:732:LYS:HD2	2.30	0.45
1:D:262:ALA:HB3	1:D:476:PRO:CG	2.44	0.45
1:D:153:ARG:HG2	1:D:229:GLN:HB2	1.99	0.45
1:A:267:TRP:CD2	1:A:341:LYS:HG3	2.51	0.45
1:E:282:ASP:HA	1:E:324:THR:HG23	1.98	0.45
1:C:48:LEU:HD23	1:C:48:LEU:N	2.31	0.45
1:C:267:TRP:CD2	1:C:341:LYS:HG3	2.52	0.45
1:C:736:LEU:C	1:C:736:LEU:HD13	2.37	0.45
1:A:735:THR:HG23	1:A:760:VAL:HG13	1.97	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:C:137:ASN:HB3	1:C:152:GLU:OE1	2.17	0.45
1:A:681:VAL:HG22	1:A:681:VAL:O	2.17	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:D:447:LEU:C	1:D:447:LEU:HD23	2.37	0.45
1:E:654:HIS:N	1:E:654:HIS:CD2	2.85	0.45
1:F:476:PRO:C	1:F:477:VAL:HG12	2.37	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:C:730:GLU:HG3	1:C:732:LYS:HZ3	1.79	0.45
1:A:123:LEU:HD13	1:A:128:ARG:CA	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:671:LEU:N	1:C:671:LEU:HD12	2.32	0.45
1:B:327:ASP:OD2	1:B:330:GLY:HA3	2.17	0.45
1:A:274:THR:CG2	1:A:276:SER:H	2.05	0.45
1:B:671:LEU:CD1	1:B:671:LEU:N	2.80	0.45
1:E:45:THR:HG23	1:E:46:TRP:CD1	2.32	0.45
1:E:196:ASN:C	1:E:197:ILE:HG12	2.37	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:E:752:GLN:HB2	1:E:759:LEU:HD11	1.98	0.45
1:D:736:LEU:HD13	1:D:737:CYS:N	2.31	0.45
1:E:190:THR:HA	1:F:223:GLU:O	2.16	0.45
1:A:264:PRO:HD3	1:A:507:PHE:CE2	2.52	0.45
1:F:379:LYS:O	1:F:380:TRP:HB3	2.16	0.45
1:D:163:TYR:HB3	1:D:502:LEU:HD13	1.98	0.45
1:F:329:GLU:H	1:F:329:GLU:CD	2.20	0.45
1:A:155:ASP:OD1	1:A:227:LYS:HE3	2.16	0.45
1:B:466:ARG:HB2	1:B:479:TRP:CH2	2.52	0.45
1:A:689:HIS:CE1	1:A:739:ARG:HH21	2.35	0.45
1:F:510:HIS:CD2	1:F:510:HIS:N	2.83	0.45
1:F:538:ARG:NH2	1:F:540:HIS:CD2	2.85	0.45
1:E:718:ARG:HB2	1:E:723:ILE:CG2	2.46	0.45
1:F:692:ASN:ND2	1:F:692:ASN:N	2.64	0.45
1:B:277:PHE:CD2	1:B:278:THR:HG23	2.52	0.45
1:A:693:LEU:HD11	1:A:716:ALA:O	2.17	0.45
1:A:290:ILE:HD13	1:A:340:LEU:HD11	1.98	0.45
1:C:273:LEU:HD13	1:C:273:LEU:C	2.37	0.45
1:C:692:ASN:ND2	5:C:3050:HOH:O	2.48	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:F:690:LEU:HD21	1:F:693:LEU:HD12	1.99	0.45
1:E:297:ASN:O	1:E:299:PRO:HD3	2.16	0.45
1:B:703:VAL:O	1:B:711:ILE:HG22	2.17	0.45
1:F:634:ARG:NH2	1:F:643:GLU:CB	2.80	0.44
1:A:476:PRO:O	1:A:477:VAL:HG13	2.17	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:D:201:MET:HE1	1:D:247:PRO:HB3	1.99	0.44
1:F:82:TYR:CD1	1:F:470:VAL:HB	2.52	0.44
1:E:731:ALA:C	1:E:732:LYS:HD2	2.37	0.44
1:C:630:LEU:O	1:C:647:SER:N	2.50	0.44
1:E:262:ALA:HB3	1:E:476:PRO:CG	2.47	0.44
1:D:278:THR:HG21	1:E:45:THR:HA	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:277:PHE:HZ	1:D:48:LEU:HD22	1.81	0.44
1:B:272:TRP:HB2	1:B:538:ARG:HA	1.98	0.44
1:B:247:PRO:HD2	5:B:3046:HOH:O	2.16	0.44
1:C:498:LEU:HD21	1:C:608:TYR:HB3	1.99	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:F:89:ASP:N	1:F:89:ASP:OD1	2.49	0.44
1:C:482:ASP:OD1	3:C:803:XYF:O2	2.33	0.44
1:D:100:TYR:HE2	1:D:113:SER:HG	1.64	0.44
1:B:631:PRO:HD2	1:B:635:TRP:CZ2	2.52	0.44
1:D:275:THR:HG23	1:D:275:THR:O	2.17	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:619:VAL:HG11	1:F:624:GLY:HA2	1.99	0.44
1:F:342:ILE:HD12	1:F:342:ILE:N	2.33	0.44
1:B:635:TRP:CZ3	1:B:664:ARG:HG2	2.53	0.44
1:B:191:GLU:HB3	1:C:222:SER: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:353:LYS:HG2	1:F:353:LYS:O	2.17	0.44
1:D:348:PRO:HG2	1:D:349:TYR:CE1	2.53	0.44
1:A:748:GLN:O	1:A:749:ASP:HB2	2.17	0.44
1:F:692:ASN:H	1:F:692:ASN:ND2	2.12	0.44
1:D:744:VAL:HG21	1:D:770:ILE:CG2	2.47	0.44
1:F:45:THR:HG23	1:F:46:TRP:CD1	2.53	0.44
1:D:749:ASP:CG	1:D:767:ALA:HB3	2.38	0.44
1:D:341:LYS:C	1:D:342:ILE:HD12	2.38	0.44
1:C:100:TYR:CD1	1:C:111:ARG:HD2	2.53	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:A:38:PRO:HG2	1:A:51:PRO:HD2	1.99	0.44
1:D:488:GLU:O	1:D:492:GLU:HG3	2.16	0.44
1:A:137:ASN:HB3	1:A:152:GLU:OE1	2.17	0.44
1:F:347:ASN:HA	1:F:444:TYR:OH	2.18	0.44
1:A:11:GLN:HB2	1:A:14:LEU:HD12	2.00	0.44
1:D:610:LEU:O	1:D:614:VAL:HG13	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:A:711:ILE:O	1:A:711:ILE:HG12	2.17	0.44
1:A:290:ILE:HD12	1:A:335:LEU:CD2	2.48	0.44
1:D:300:LEU:HD13	1:D:301:HIS:H	1.82	0.44
1:E:744:VAL:HG23	1:E:772:LEU:HA	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:201:MET:HE3	1:B:247:PRO:HB3	2.00	0.44
1:E:489:SER:HA	1:E:492:GLU:CD	2.38	0.44
1:C:156:LEU:HD11	1:C:228:VAL:HG23	1.98	0.44
1:E:490:MET:HE3	1:E:620:PHE:CD1	2.53	0.44
1:D:69:ILE:HG12	1:D:150:MET:HE1	1.99	0.44
1:B:98:GLU:H	1:B:98:GLU:CD	2.21	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: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:B:635:TRP:CH2	1:B:664:ARG:HG2	2.53	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:E:554:GLU:O	1:E:558:VAL:HG23	2.17	0.43
1:A:763:PRO:HB3	1:A:768:LEU:HD12	1.99	0.43
1:F:82:TYR:CB	1:F:84:LEU:HD13	2.47	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
1:E:163:TYR:HB3	1:E:502:LEU:HD13	2.01	0.43
1:A:327:ASP:OD2	1:A:330:GLY:HA3	2.19	0.43
1:F:359:GLU:OE2	1:F:363:LYS:NZ	2.49	0.43
1:B:532:LEU:O	1:B:566:LYS:HD2	2.18	0.43
1:A:25:VAL:HG21	1:A:114:LYS:HE2	2.00	0.43
1:A:300:LEU:HD12	1:A:340:LEU:CD2	2.48	0.43
1:C:165:LEU:HD13	1:C:179:VAL:CG2	2.48	0.43
1:D:522:HIS:CD2	1:D:622:GLU:HG3	2.53	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:89:ASP:N	1:C:89:ASP:OD1	2.51	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:C:575:ARG:CZ	1:C:579:ARG:HH12	2.31	0.43
1:E:165:LEU:HA	1:E:197:ILE:O	2.18	0.43
1:E:128:ARG:HH22	1:E:131:GLY:CA	2.31	0.43
1:D:290:ILE:CD1	1:D:335:LEU:HD22	2.49	0.43
1:F:509:SER:HB2	1:F:536:HIS:HB2	2.00	0.43
1:B:516:GLU:O	1:B:517:ASN:HB2	2.19	0.43
1:F:275:THR:HG22	1:F:303:PHE:HZ	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:262:ALA:HB3	1:A:476:PRO:CD	2.49	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:D:32:MET:HB2	1:D:32:MET:HE2	1.71	0.43
1:A:547:VAL:HA	1:A:548:PRO:HD3	1.91	0.43
1:F:164:GLY:O	1:F:165:LEU:HB2	2.18	0.43
1:A:429:ASP:OD1	1:A:431:SER:OG	2.30	0.43
1:C:70:GLU:HB3	1:C:236:TYR:HB2	2.01	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: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:E:164:GLY:O	1:E:165:LEU:HB2	2.18	0.43
1:E:287:ASN:ND2	1:E:334:ARG:NH2	2.64	0.43
1:E:302:VAL:HG22	1:E:341:LYS:HB2	2.00	0.43
1:C:226:SER:O	1:C:227:LYS:HG3	2.19	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:A:476:PRO:C	1:A:477:VAL:HG13	2.39	0.43
1:C:525:LYS:HB3	1:C:656:PHE:CD1	2.54	0.43
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:D:765:GLY:O	1:D:767:ALA:N	2.50	0.43
1:D:576:GLU:OE2	1:D:579:ARG:NH1	2.52	0.43
1:C:314:GLN:HB3	1:C:354:SER:HB2	2.00	0.43
1:E:310:MET:SD	1:E:316:CYS:HA	2.59	0.43
1:A:384:LEU:C	1:A:384:LEU:HD23	2.38	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:F:723:ILE:N	1:F:723:ILE:HD12	2.34	0.42
1:D:358:LYS:HE2	1:D:362:GLU:OE2	2.19	0.42
1:F:681:VAL:HG12	2:F:3005:SO4:S	2.60	0.42
1:C:70:GLU:OE1	1:C:73:GLN:HG2	2.18	0.42
1:C:45:THR:HG23	1:C:46:TRP:CD1	2.53	0.42
1:D:354:SER:HA	1:D:355:PRO:HD3	1.91	0.42
1:E:318:PHE:HB2	1:E:401:LYS:HD2	2.00	0.42
1:A:652:GLN:NE2	1:A:654:HIS:NE2	2.66	0.42
1:F:406:VAL:HG11	1:F:455:THR:HB	2.01	0.42
1:F:98:GLU:HG3	1:F:98:GLU:O	2.19	0.42
1:D:264:PRO:HD3	1:D:507:PHE:CE2	2.54	0.42
1:C:274:THR:HG23	1:C:276:SER:N	2.34	0.42
1:D:273:LEU:HD13	1:D:274:THR:N	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:31:GLU:HG2	1:C:58:PHE:CB	2.49	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: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:A:300:LEU:HD12	1:A:340:LEU:HD21	2.02	0.42
1:F:273:LEU:HD22	1:F:274:THR:H	1.83	0.42
1:A:367:LEU:CD1	1:A:425:VAL:HG21	2.49	0.42
1:D:540:HIS:CA	1:D:546:ARG:HD2	2.50	0.42
1:C:748:GLN:HB2	1:C:769:THR:HB	2.01	0.42
1:E:379:LYS:O	1:E:380:TRP:HB3	2.19	0.42
1:F:691:PHE:O	1:F:692:ASN:C	2.57	0.42
1:A:414:LYS:NZ	1:A:538:ARG:HH12	2.15	0.42
1:C:123:LEU:HA	1:C:127:GLU:O	2.19	0.42
1:E:683:HIS:HD2	1:E:730:GLU:HG2	1.84	0.42
1:B:201:MET:HE1	1:B:247:PRO:HB3	2.02	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:E:358:LYS:HG2	1:E:362:GLU:OE2	2.19	0.42
1:C:212:HIS:HA	1:C:213:PRO:HD3	1.88	0.42
1:A:544:SER:O	1:A:546:ARG:NH1	2.53	0.42
1:F:293:MET:CE	1:F:300:LEU:HD23	2.50	0.42
1:C:356:VAL:HG11	1:C:397:TRP:HH2	1.85	0.42
1:C:341:LYS:C	1:C:342:ILE:HD12	2.40	0.42
1:D:526:ARG:HD2	1:D:619:VAL:HB	2.00	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:A:37:ALA:HA	1:A:38:PRO:HD3	1.79	0.42
1:F:693:LEU:HD11	1:F:716:ALA:O	2.18	0.42
1:C:43:GLU:HB3	1:C:45:THR:HG22	2.01	0.42
1:A:354:SER:HA	1:A:355:PRO:HD3	1.89	0.42
1:C:635:TRP:CH2	1:C:664:ARG:HB3	2.55	0.42
1:B:668:LEU:CD2	1:B:714:LEU:HD12	2.29	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:C:164:GLY:O	1:C:165:LEU:HB2	2.20	0.42
1:B:123:LEU:CD2	1:B:123:LEU:N	2.82	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:D:58:PHE:N	1:D:58:PHE:CD1	2.88	0.42
1:D:69:ILE:HG12	1:D:150:MET:CE	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:619:VAL:HG11	1:D:624:GLY:HA2	2.01	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:F:753:ALA:O	1:F:759:LEU:HD12	2.20	0.42
1:E:58:PHE:CD1	1:E:58:PHE:N	2.88	0.42
1:B:744:VAL:CG2	1:B:772:LEU:HA	2.50	0.42
1:A:164:GLY:O	1:A:165:LEU:HB2	2.20	0.42
1:A:735:THR:CG2	1:A:736:LEU:N	2.81	0.42
1:D:497:GLY:O	1:D:500:ILE:HG22	2.20	0.42
1:A:424:ASP:N	1:A:424:ASP:OD2	2.50	0.42
1:F:311:LYS:HE3	1:F:314:GLN:CD	2.40	0.42
1:C:736:LEU:CD1	1:C:738:LEU:HD23	2.50	0.42
1:F:80:PRO:HD3	1:F:431:SER:HB3	2.01	0.42
1:E:670:ALA:C	1:E:671:LEU:HD12	2.40	0.42
1:E:565:LEU:O	1:E:569:MET:HG3	2.19	0.42
1:C:730:GLU:HG3	1:C:732:LYS:HZ2	1.85	0.42
1:E:334:ARG:O	1:E:337:ALA:HB3	2.20	0.42
1:B:497:GLY:O	1:B:500:ILE:HG22	2.20	0.42
1:D:588:MET:HG3	1:D:608:TYR:CD1	2.54	0.42
1:B:414:LYS:HZ2	1:B:538:ARG:HH12	1.68	0.42
1:E:17:ILE:HG12	1:E:139:TYR:HB3	2.02	0.42
1:C:182:TRP:CE3	1:C:215:CYS:HB2	2.55	0.42
1:D:344:VAL:HG22	1:D:410:VAL:HG11	2.02	0.42
1:C:770:ILE:HD12	1:C:770:ILE:C	2.40	0.42
1:E:214:GLN:HE22	1:E:232:VAL:HG21	1.85	0.41
1:F:634:ARG:HH21	1:F:643:GLU:CB	2.24	0.41
1:A:747:LEU:HD23	1:A:747:LEU:C	2.40	0.41
1:C:171:ALA:O	1:C:174:ARG:NH2	2.39	0.41
1:B:195:LYS:HB3	1:B:468:ALA:HB3	2.00	0.41
1:D:262:ALA:HB3	1:D:476:PRO:CD	2.50	0.41
1:B:485:ALA:HB1	1:B:519:ALA:CB	2.48	0.41
1:E:37:ALA:HA	1:E:38:PRO:HD3	1.87	0.41
1:E:314:GLN:HB3	1:E:317:ASP:OD2	2.19	0.41
1:B:730:GLU:HG3	1:B:732:LYS:HZ2	1.85	0.41
1:D:634:ARG:CZ	1:D:645:ASP:OD1	2.67	0.41
1:B:405:LEU:O	1:B:410:VAL:HG23	2.20	0.41
1:B:145:ASN:OD1	1:B:147:ARG:HB2	2.19	0.41
1:A:752:GLN:OE1	1:A:759:LEU:HD21	2.20	0.41
1:A:300:LEU:CD1	1:A:340:LEU:HD22	2.51	0.41
1:C:367:LEU:HD11	1:C:425:VAL:CG2	2.46	0.41
1:F:419:GLU:H	1:F:419:GLU:CD	2.23	0.41
1:A:191:GLU:OE1	1:D:223:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:182:TRP:CE3	1:B:215:CYS:HB2	2.55	0.41
1:C:580:ALA:HA	1:C:585:THR:O	2.19	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:F:273:LEU:HD12	1:F:303:PHE:HE1	1.85	0.41
1:F:749:ASP:CG	1:F:767:ALA:HB3	2.41	0.41
1:C:17:ILE:HG12	1:C:139:TYR:HB3	2.02	0.41
1:F:522:HIS:CG	1:F:622:GLU:HG3	2.56	0.41
1:E:17:ILE:CG1	1:E:139:TYR:HB3	2.51	0.41
1:D:21:GLN:HE22	1:D:41:VAL:H	1.68	0.41
1:B:634:ARG:HG2	1:B:692:ASN:OD1	2.20	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:F:108:LEU:HD22	1:F:243:ASP:HB2	2.02	0.41
1:C:36:ALA:O	1:C:52:LEU:HD22	2.20	0.41
1:D:293:MET:HE3	1:D:300:LEU:HD23	2.01	0.41
1:D:293:MET:HE2	1:D:300:LEU:HD23	2.02	0.41
1:E:569:MET:CB	1:E:573:LEU:HD22	2.50	0.41
1:E:547:VAL:CG2	1:E:550:ALA:HB2	2.50	0.41
1:E:634:ARG:HH21	1:E:643:GLU:HB3	1.86	0.41
1:B:190:THR:HA	1:C:223:GLU:O	2.21	0.41
1:E:296:ARG:O	1:E:560:ARG:NH1	2.54	0.41
1:D:39:ARG:HD2	5:D:3056:HOH:O	2.20	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:731:ALA:O	1:A:732:LYS:HD2	2.20	0.41
1:D:745:ASN:HB3	1:D:771:THR:O	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:A:307:CYS:HB3	1:A:315:TRP:CZ2	2.56	0.41
1:C:526:ARG:NH2	1:C:624:GLY:HA2	2.35	0.41
1:E:82:TYR:CD1	1:E:470:VAL:HB	2.55	0.41
1:E:173:VAL:HG21	1:E:603:TYR:CD1	2.56	0.41
1:A:770:ILE:HD11	1:A:772:LEU:CD2	2.50	0.41
1:E:333:ARG:NH1	1:E:336:LYS:HE3	2.36	0.41
1:A:336:LYS:CG	1:A:342:ILE:HD13	2.50	0.41
1:C:453:LYS:HG3	1:C:458:GLU:HA	2.02	0.41
1:A:681:VAL:HG23	1:A:683:HIS:CE1	2.56	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:345:TRP:O	1:E:346:ILE:CG2	2.69	0.41
1:B:552:ASP:OD1	1:B:555:SER:N	2.38	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:472:ALA:HB1	5:B:3074:HOH:O	2.21	0.41
1:C:143:THR:O	1:C:143:THR:HG22	2.20	0.41
1:E:80:PRO:HD2	1:E:435:LYS:HB2	2.01	0.41
1:A:548:PRO:CG	1:A:559:VAL:HG21	2.48	0.41
1:E:277:PHE:HB3	1:E:542:SER:HA	2.02	0.41
1:B:635:TRP:HB3	1:B:662:TYR:HB3	2.03	0.41
1:B:439:HIS:NE2	1:B:443:ILE:HD11	2.34	0.41
1:F:770:ILE:HD11	1:F:772:LEU:HD23	2.02	0.41
1:B:252:ASP:HA	1:B:583:ARG:O	2.21	0.41
1:E:275:THR:HG22	1:E:303:PHE:HZ	1.86	0.41
1:B:718:ARG:CB	1:B:723:ILE:HG22	2.51	0.41
1:B:670:ALA:C	1:B:671:LEU:HD12	2.41	0.41
1:F:485:ALA:CB	1:F:519:ALA:HB2	2.31	0.41
1:D:171:ALA:O	1:D:174:ARG:NH2	2.43	0.41
1:B:583:ARG:HD3	5:B:3057:HOH:O	2.19	0.41
1:D:67:VAL:O	1:D:238:GLU:HA	2.21	0.41
1:B:639:TRP:HE1	1:B:640:HIS:CE1	2.38	0.41
1:D:533:LEU:HD12	1:D:533:LEU:HA	1.94	0.41
1:A:521:ALA:O	1:A:525:LYS:HE3	2.20	0.41
1:F:631:PRO:O	1:F:646:GLY:HA3	2.20	0.41
1:F:547:VAL:HA	1:F:548:PRO:HD3	1.96	0.41
1:E:314:GLN:HB3	1:E:354:SER:HB2	2.01	0.41
1:F:37:ALA:HA	1:F:38:PRO:HD3	1.81	0.41
1:F:82:TYR:CE1	1:F:470:VAL:HB	2.56	0.41
1:C:11:GLN:HA	1:C:12:PRO:HD3	1.97	0.41
1:E:414:LYS:HZ2	1:E:538:ARG:HH12	1.69	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:D:155:ASP:HB3	5:D:3094:HOH:O	2.21	0.41
1:C:37:ALA:HA	1:C:38:PRO:HD3	1.78	0.41
1:E:447:LEU:O	1:E:451:VAL:HG23	2.20	0.41
1:E:153:ARG:HG2	1:E:229:GLN:HB2	2.02	0.41
1:C:509:SER:OG	1:C:510:HIS:N	2.54	0.41
1:A:306:ASP:O	1:A:309:TRP:HD1	2.04	0.41
1:B:633:GLY:O	1:B:646:GLY:N	2.53	0.41
1:E:327:ASP:OD2	1:E:330:GLY:HA3	2.20	0.41
1:A:615:MET:SD	1:A:615:MET:C	3.00	0.41
1:E:716:ALA:HA	1:E:724:THR:O	2.21	0.41
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:681:VAL:HG23	1:D:683:HIS:CE1	2.56	0.40
1:A:11:GLN:HB2	1:A:14:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:120:LEU:HD23	1:B:121:ASP:N	2.36	0.40
1:D:261:PRO:O	1:D:581:ASN:HA	2.21	0.40
1:D:308:PHE:CE1	1:D:315:TRP:HZ2	2.40	0.40
1:D:277:PHE:CD2	1:D:278:THR:HG23	2.56	0.40
1:F:635:TRP:CZ3	1:F:664:ARG:HG2	2.56	0.40
1:F:761:VAL:HG11	1:F:768:LEU:HD11	2.03	0.40
1:C:349:TYR:HB3	1:C:384:LEU:HD21	2.03	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:719:THR:HG22	1:E:722:THR:O	2.22	0.40
1:E:610:LEU:O	1:E:614:VAL:HG13	2.20	0.40
1:B:601:CYS:HA	1:B:604:LEU:HG	2.03	0.40
1:B:122:PHE:CE1	1:B:241:VAL:HG21	2.56	0.40
1:F:67:VAL:O	1:F:238:GLU:HA	2.21	0.40
1:B:718:ARG:HH21	1:B:772:LEU:HD12	1.86	0.40
1:B:690:LEU:O	1:B:739:ARG:HB2	2.21	0.40
1:A:747:LEU:HD11	1:A:761:VAL:HG13	2.02	0.40
1:E:300:LEU:HD12	1:E:340:LEU:CD2	2.52	0.40
1:C:18:HIS:HB2	1:C:20:LEU:CD2	2.51	0.40
1:E:512:ILE:HB	1:E:539:LEU:HD23	2.02	0.40
1:D:772:LEU:CD2	1:D:772:LEU:H	2.34	0.40
1:C:310:MET:SD	1:C:316:CYS:HA	2.61	0.40
1:C:274:THR:HG22	1:C:539:LEU:O	2.21	0.40
1:F:670:ALA:HB2	1:F:701:CYS:SG	2.61	0.40
1:B:381:GLN:O	1:B:384:LEU:HB2	2.21	0.40
1:D:282:ASP:HA	1:D:324:THR:HG23	2.04	0.40
1:F:533:LEU:HD23	1:F:659:LEU:HD11	2.03	0.40
1:D:634:ARG:NH2	1:D:634:ARG:HG3	2.35	0.40
1:C:598:ASP:HA	1:C:599:PRO:HD2	1.94	0.40
1:F:273:LEU:CB	1:F:300:LEU:HD21	2.45	0.40
1:A:635:TRP:HB3	1:A:662:TYR:HB3	2.03	0.40
1:F:31:GLU:OE1	1:F:56:ARG:HD3	2.22	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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	771/778 (99%)	716 (93%)	45 (6%)	10 (1%)	18	13
1	B	771/778 (99%)	712 (92%)	44 (6%)	15 (2%)	12	7
1	C	771/778 (99%)	716 (93%)	47 (6%)	8 (1%)	22	18
1	D	771/778 (99%)	709 (92%)	47 (6%)	15 (2%)	12	7
1	E	771/778 (99%)	709 (92%)	52 (7%)	10 (1%)	18	13
1	F	771/778 (99%)	709 (92%)	51 (7%)	11 (1%)	16	12
All	All	4626/4668 (99%)	4271 (92%)	286 (6%)	69 (2%)	15	10

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	44	53
1	B	659/665 (99%)	643 (98%)	16 (2%)	61	73
1	C	659/665 (99%)	630 (96%)	29 (4%)	39	45
1	D	659/665 (99%)	630 (96%)	29 (4%)	39	45
1	E	659/665 (99%)	634 (96%)	25 (4%)	44	53
1	F	659/665 (99%)	635 (96%)	24 (4%)	47	56
All	All	3954/3990 (99%)	3806 (96%)	148 (4%)	45	54

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains 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 carbohydrates 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	A	3012	-	4,4,4	3.43	2 (50%)	6,6,6	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	3013	-	4,4,4	3.47	2 (50%)	6,6,6	0.91	0
3	XYF	A	801	1	9,10,11	2.04	3 (33%)	10,14,16	0.64	0
4	MPO	B	2001	-	13,13,13	1.91	2 (15%)	17,17,17	2.79	6 (35%)
2	SO4	B	3008	-	4,4,4	3.41	2 (50%)	6,6,6	0.94	0
2	SO4	B	3010	-	4,4,4	3.47	2 (50%)	6,6,6	0.95	0
3	XYF	B	802	1	9,10,11	2.02	3 (33%)	10,14,16	0.67	0
4	MPO	C	2002	-	13,13,13	2.00	2 (15%)	17,17,17	2.72	6 (35%)
2	SO4	C	3007	-	4,4,4	3.41	2 (50%)	6,6,6	0.95	0
2	SO4	C	3011	-	4,4,4	3.38	2 (50%)	6,6,6	0.96	0
3	XYF	C	803	1	9,10,11	2.03	3 (33%)	10,14,16	0.69	0
4	MPO	D	2003	-	13,13,13	1.85	2 (15%)	17,17,17	2.78	6 (35%)
2	SO4	D	3004	-	4,4,4	3.53	2 (50%)	6,6,6	0.90	0
4	MPO	E	2004	-	13,13,13	1.85	2 (15%)	17,17,17	2.76	6 (35%)
2	SO4	E	3006	-	4,4,4	3.47	2 (50%)	6,6,6	0.91	0
3	XYF	E	804	1	9,10,11	2.01	3 (33%)	10,14,16	0.61	0
2	SO4	F	3001	-	4,4,4	3.42	2 (50%)	6,6,6	0.92	0
2	SO4	F	3002	-	4,4,4	3.43	2 (50%)	6,6,6	0.94	0
2	SO4	F	3003	-	4,4,4	3.50	2 (50%)	6,6,6	0.96	0
2	SO4	F	3005	-	4,4,4	3.43	2 (50%)	6,6,6	0.90	0
2	SO4	F	3009	-	4,4,4	3.46	2 (50%)	6,6,6	0.94	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
2	SO4	A	3012	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3013	-	-	0/0/0/0	0/0/0/0
3	XYF	A	801	1	-	0/0/17/20	0/1/1/1
4	MPO	B	2001	-	-	0/7/15/15	0/1/1/1
2	SO4	B	3008	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3010	-	-	0/0/0/0	0/0/0/0
3	XYF	B	802	1	-	0/0/17/20	0/1/1/1
4	MPO	C	2002	-	-	0/7/15/15	0/1/1/1
2	SO4	C	3007	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3011	-	-	0/0/0/0	0/0/0/0
3	XYF	C	803	1	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPO	D	2003	-	-	0/7/15/15	0/1/1/1
2	SO4	D	3004	-	-	0/0/0/0	0/0/0/0
4	MPO	E	2004	-	-	0/7/15/15	0/1/1/1
2	SO4	E	3006	-	-	0/0/0/0	0/0/0/0
3	XYF	E	804	1	-	0/0/17/20	0/1/1/1
2	SO4	F	3001	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3002	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3003	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3005	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3009	-	-	0/0/0/0	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2002	MPO	C1-S1	5.86	1.86	1.77
4	B	2001	MPO	C1-S1	5.49	1.85	1.77
4	D	2003	MPO	C1-S1	5.26	1.85	1.77
4	E	2004	MPO	C1-S1	5.15	1.85	1.77
2	D	3004	SO4	O1-S	4.96	1.63	1.47
2	F	3003	SO4	O3-S	-4.95	1.30	1.47
2	D	3004	SO4	O3-S	-4.91	1.30	1.47
2	A	3013	SO4	O1-S	4.90	1.63	1.47
2	F	3009	SO4	O1-S	4.90	1.63	1.47
2	B	3010	SO4	O1-S	4.90	1.63	1.47
2	F	3003	SO4	O1-S	4.88	1.63	1.47
2	A	3012	SO4	O1-S	4.87	1.62	1.47
2	E	3006	SO4	O1-S	4.86	1.62	1.47
2	E	3006	SO4	O3-S	-4.85	1.30	1.47
2	B	3008	SO4	O1-S	4.85	1.62	1.47
2	B	3010	SO4	O3-S	-4.83	1.30	1.47
2	F	3002	SO4	O1-S	4.83	1.62	1.47
2	F	3001	SO4	O1-S	4.81	1.62	1.47
2	F	3005	SO4	O1-S	4.81	1.62	1.47
2	A	3013	SO4	O3-S	-4.81	1.30	1.47
2	F	3005	SO4	O3-S	-4.81	1.30	1.47
2	F	3009	SO4	O3-S	-4.80	1.31	1.47
2	F	3001	SO4	O3-S	-4.78	1.31	1.47
2	C	3007	SO4	O3-S	-4.78	1.31	1.47
2	F	3002	SO4	O3-S	-4.78	1.31	1.47
2	C	3007	SO4	O1-S	4.76	1.62	1.47
2	A	3012	SO4	O3-S	-4.76	1.31	1.47
2	C	3011	SO4	O3-S	-4.76	1.31	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3008	SO4	O3-S	-4.70	1.31	1.47
2	C	3011	SO4	O1-S	4.69	1.62	1.47
3	B	802	XYF	O5-C5	4.58	1.44	1.40
3	C	803	XYF	O5-C5	4.57	1.44	1.40
3	A	801	XYF	O5-C5	4.53	1.44	1.40
3	E	804	XYF	O5-C5	4.50	1.44	1.40
3	E	804	XYF	F5-C5	-3.13	1.35	1.39
3	C	803	XYF	F5-C5	-3.10	1.35	1.39
3	A	801	XYF	F5-C5	-3.08	1.35	1.39
3	B	802	XYF	F5-C5	-3.08	1.35	1.39
3	A	801	XYF	C4-C5	2.52	1.53	1.52
3	C	803	XYF	C4-C5	2.37	1.53	1.52
3	E	804	XYF	C4-C5	2.31	1.53	1.52
4	B	2001	MPO	C4-N1	2.26	1.53	1.47
3	B	802	XYF	C4-C5	2.25	1.53	1.52
4	E	2004	MPO	C4-N1	2.23	1.53	1.47
4	C	2002	MPO	C4-N1	2.23	1.53	1.47
4	D	2003	MPO	C4-N1	2.12	1.52	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	-7.80	103.17	113.24
4	E	2004	MPO	C2-C1-S1	-7.62	103.41	113.24
4	B	2001	MPO	C2-C1-S1	-7.51	103.56	113.24
4	C	2002	MPO	C2-C1-S1	-7.20	103.95	113.24
4	B	2001	MPO	O1-S1-C1	5.12	111.19	106.81
4	C	2002	MPO	O1-S1-C1	4.90	111.01	106.81
4	E	2004	MPO	O1-S1-C1	4.59	110.75	106.81
4	D	2003	MPO	O1-S1-C1	4.51	110.67	106.81
4	E	2004	MPO	O2-S1-C1	4.16	110.38	106.81
4	C	2002	MPO	O2-S1-C1	4.14	110.36	106.81
4	B	2001	MPO	O2-S1-C1	4.06	110.29	106.81
4	D	2003	MPO	O2-S1-C1	3.98	110.22	106.81
4	B	2001	MPO	C3-C2-C1	-3.25	104.76	112.42
4	E	2004	MPO	C3-C2-C1	-3.16	104.96	112.42
4	D	2003	MPO	C3-C2-C1	-3.12	105.06	112.42
4	C	2002	MPO	C3-C2-C1	-3.08	105.17	112.42
4	D	2003	MPO	C5-C4-N1	-2.41	106.51	110.04
4	C	2002	MPO	C5-C4-N1	-2.37	106.57	110.04
4	E	2004	MPO	C2-C3-N1	-2.26	108.04	113.94
4	D	2003	MPO	C2-C3-N1	-2.25	108.06	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	MPO	C2-C3-N1	-2.24	108.08	113.94
4	B	2001	MPO	C5-C4-N1	-2.23	106.78	110.04
4	E	2004	MPO	C5-C4-N1	-2.22	106.78	110.04
4	C	2002	MPO	C2-C3-N1	-2.17	108.27	113.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.10	16 (2%)	60	61	16, 28, 48, 76	0
1	B	773/778 (99%)	0.17	40 (5%)	26	26	20, 36, 61, 82	0
1	C	773/778 (99%)	-0.06	19 (2%)	54	55	17, 29, 50, 72	0
1	D	773/778 (99%)	0.15	47 (6%)	21	20	17, 31, 63, 84	0
1	E	773/778 (99%)	-0.00	29 (3%)	38	39	18, 32, 55, 90	0
1	F	773/778 (99%)	0.09	32 (4%)	35	36	19, 30, 55, 77	0
All	All	4638/4668 (99%)	0.04	183 (3%)	37	38	16, 31, 56, 90	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	767	ALA	8.3
1	F	719	THR	7.7
1	B	766	ASN	7.4
1	E	46	TRP	7.0
1	E	766	ASN	6.9
1	D	277	PHE	6.7
1	C	766	ASN	6.6
1	D	278	THR	6.4
1	E	43	GLU	6.3
1	D	382	PRO	6.0
1	B	765	GLY	5.9
1	F	766	ASN	5.9
1	D	540	HIS	5.9
1	D	545	TYR	5.9
1	D	766	ASN	5.7
1	C	765	GLY	5.1
1	D	279	THR	5.1
1	A	766	ASN	5.0
1	D	546	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	42	ARG	4.9
1	D	541	GLY	4.9
1	D	765	GLY	4.9
1	E	765	GLY	4.7
1	F	748	GLN	4.6
1	F	772	LEU	4.5
1	B	719	THR	4.5
1	A	765	GLY	4.4
1	D	281	TYR	4.4
1	E	47	GLN	4.3
1	F	770	ILE	4.3
1	C	767	ALA	4.1
1	F	765	GLY	4.1
1	A	719	THR	4.0
1	B	744	VAL	4.0
1	A	768	LEU	4.0
1	C	748	GLN	3.9
1	D	275	THR	3.9
1	D	380	TRP	3.8
1	D	477	VAL	3.7
1	D	747	LEU	3.6
1	F	768	LEU	3.6
1	E	767	ALA	3.5
1	D	276	SER	3.5
1	B	764	GLN	3.5
1	B	407	ALA	3.5
1	B	753	ALA	3.5
1	B	323	LEU	3.5
1	E	44	ARG	3.4
1	D	767	ALA	3.4
1	B	768	LEU	3.4
1	E	49	ASP	3.4
1	D	764	GLN	3.4
1	B	29	ASP	3.4
1	F	767	ALA	3.4
1	D	763	PRO	3.4
1	D	743	LYS	3.3
1	B	736	LEU	3.3
1	B	742	VAL	3.3
1	C	770	ILE	3.3
1	A	477	VAL	3.2
1	B	743	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	88	GLN	3.2
1	F	749	ASP	3.2
1	B	545	TYR	3.1
1	E	117	PHE	3.1
1	B	88	GLN	3.1
1	E	477	VAL	3.1
1	E	40	ASP	3.1
1	B	722	THR	3.1
1	C	719	THR	3.1
1	F	738	LEU	3.0
1	B	477	VAL	3.0
1	B	745	ASN	3.0
1	B	723	ILE	3.0
1	B	772	LEU	2.9
1	D	542	SER	2.9
1	C	772	LEU	2.9
1	B	325	PHE	2.9
1	D	289	PHE	2.9
1	F	88	GLN	2.9
1	D	88	GLN	2.9
1	A	772	LEU	2.9
1	C	773	HIS	2.9
1	D	383	GLY	2.9
1	D	750	GLY	2.9
1	D	381	GLN	2.9
1	F	747	LEU	2.8
1	D	748	GLN	2.8
1	E	723	ILE	2.8
1	A	744	VAL	2.8
1	B	333	ARG	2.8
1	B	337	ALA	2.8
1	D	742	VAL	2.8
1	F	695	ASP	2.8
1	D	762	LYS	2.8
1	E	719	THR	2.8
1	B	738	LEU	2.8
1	D	280	ASN	2.7
1	D	543	LYS	2.7
1	E	706	ALA	2.7
1	F	724	THR	2.7
1	A	88	GLN	2.7
1	D	753	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	768	LEU	2.6
1	F	545	TYR	2.6
1	B	759	LEU	2.6
1	B	295	GLU	2.6
1	E	764	GLN	2.6
1	C	744	VAL	2.5
1	C	669	LEU	2.5
1	D	517	ASN	2.5
1	B	770	ILE	2.5
1	C	88	GLN	2.5
1	E	89	ASP	2.5
1	A	767	ALA	2.5
1	D	306	ASP	2.5
1	D	759	LEU	2.5
1	D	745	ASN	2.5
1	B	762	LYS	2.4
1	D	378	ASP	2.4
1	F	745	ASN	2.4
1	E	41	VAL	2.4
1	B	549	TRP	2.4
1	D	513	GLY	2.4
1	F	759	LEU	2.4
1	E	45	THR	2.4
1	B	763	PRO	2.4
1	E	743	LYS	2.3
1	D	333	ARG	2.3
1	A	721	ASN	2.3
1	E	745	ASN	2.3
1	E	39	ARG	2.3
1	C	756	GLU	2.3
1	B	338	LYS	2.3
1	C	768	LEU	2.3
1	B	756	GLU	2.3
1	F	754	GLU	2.3
1	F	756	GLU	2.3
1	C	46	TRP	2.3
1	E	76	LEU	2.3
1	D	723	ILE	2.3
1	F	547	VAL	2.2
1	D	544	SER	2.2
1	A	742	VAL	2.2
1	C	477	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	746	GLY	2.2
1	B	290	ILE	2.2
1	F	723	ILE	2.2
1	E	772	LEU	2.2
1	C	764	GLN	2.2
1	A	743	LYS	2.2
1	B	327	ASP	2.2
1	F	742	VAL	2.2
1	D	514	GLY	2.2
1	B	748	GLN	2.2
1	F	550	ALA	2.2
1	D	483	CYS	2.2
1	C	745	ASN	2.2
1	D	29	ASP	2.2
1	B	91	LYS	2.1
1	E	98	GLU	2.1
1	D	307	CYS	2.1
1	F	753	ALA	2.1
1	B	761	VAL	2.1
1	B	319	GLU	2.1
1	C	98	GLU	2.1
1	E	289	PHE	2.1
1	F	289	PHE	2.1
1	A	99	ARG	2.1
1	E	77	ASN	2.1
1	F	515	PHE	2.1
1	A	76	LEU	2.1
1	D	749	ASP	2.1
1	F	46	TRP	2.1
1	A	91	LYS	2.1
1	A	100	TYR	2.1
1	C	100	TYR	2.1
1	F	29	ASP	2.1
1	F	539	LEU	2.0
1	B	476	PRO	2.0
1	F	762	LYS	2.0
1	F	98	GLU	2.0
1	E	52	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	F	3009	5/5	0.20	9.43	91,91,92,92	0
2	SO4	F	3001	5/5	0.21	7.72	91,91,91,92	0
2	SO4	C	3011	5/5	0.28	4.92	105,106,106,106	0
2	SO4	C	3007	5/5	0.21	4.27	75,76,76,77	0
2	SO4	A	3012	5/5	0.18	3.35	87,87,88,88	0
2	SO4	E	3006	5/5	0.16	3.14	84,84,85,85	0
3	XYF	E	804	10/11	0.23	2.04	25,26,27,29	10
4	MPO	E	2004	13/13	0.15	1.94	53,55,57,58	0
2	SO4	F	3003	5/5	0.17	1.78	67,68,69,69	0
3	XYF	C	803	10/11	0.16	1.60	33,36,38,40	0
2	SO4	D	3004	5/5	0.17	1.32	75,75,75,75	0
2	SO4	F	3002	5/5	0.17	1.13	76,77,77,78	0
4	MPO	D	2003	13/13	0.20	1.03	53,57,63,63	0
4	MPO	B	2001	13/13	0.17	0.97	68,68,69,69	0
2	SO4	F	3005	5/5	0.15	0.88	58,58,59,59	0
4	MPO	C	2002	13/13	0.15	0.86	52,57,61,62	0
2	SO4	B	3008	5/5	0.16	0.66	72,72,72,73	0
2	SO4	B	3010	5/5	0.20	0.58	88,89,89,90	0
2	SO4	A	3013	5/5	0.12	0.45	77,77,78,78	0
3	XYF	B	802	10/11	0.14	0.34	37,41,43,45	0
3	XYF	A	801	10/11	0.08	-1.38	35,36,38,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.