



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:05 PM GMT

PDB ID : 1WE5
Title : Crystal Structure of Alpha-Xylosidase from Escherichia coli
Authors : Ose, T.; Kitamura, M.; Okuyama, M.; Mori, H.; Kimura, A.; Watanabe, N.; Yao, M.; Tanaka, I.
Deposited on : 2004-05-24
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

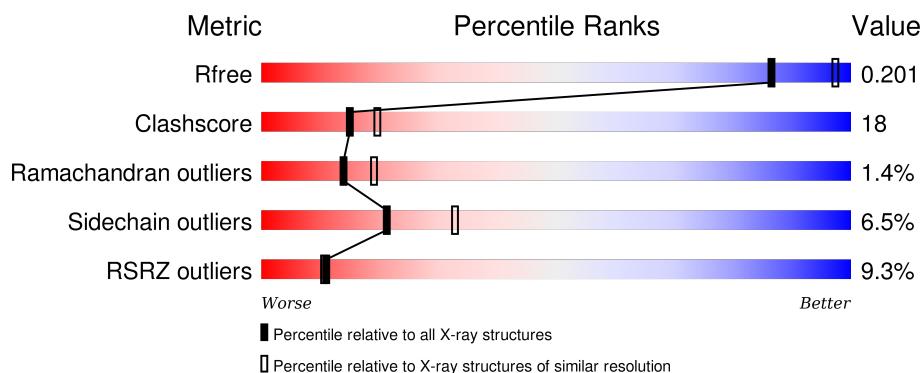
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	772	<div> <div>11%</div> <div>68% 28% .</div> </div>
1	B	772	<div> <div>9%</div> <div>65% 29% . . .</div> </div>
1	C	772	<div> <div>6%</div> <div>65% 28% 5% .</div> </div>
1	D	772	<div> <div>8%</div> <div>66% 28% . .</div> </div>
1	E	772	<div> <div>10%</div> <div>64% 30% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	772	<div><div></div><div>10%</div><div>68%</div><div>27%</div><div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 37302 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	772	Total	C	N	O	S	Se	0	0	0
			6222	3975	1068	1147	13	19			
1	B	760	Total	C	N	O	S	Se	0	0	0
			6121	3909	1051	1129	13	19			
1	C	756	Total	C	N	O	S	Se	0	0	0
			6093	3891	1047	1123	13	19			
1	D	757	Total	C	N	O	S	Se	0	0	0
			6096	3892	1047	1125	13	19			
1	E	755	Total	C	N	O	S	Se	0	0	0
			6086	3887	1045	1122	13	19			
1	F	757	Total	C	N	O	S	Se	0	0	0
			6094	3891	1047	1124	13	19			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	593	MSE	MET	MODIFIED RESIDUE	UNP P31434

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Chain	Residue	Modelled	Actual	Comment	Reference
A	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
A	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
B	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
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C	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
C	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	32	MSE	MET	MODIFIED RESIDUE	UNP P31434

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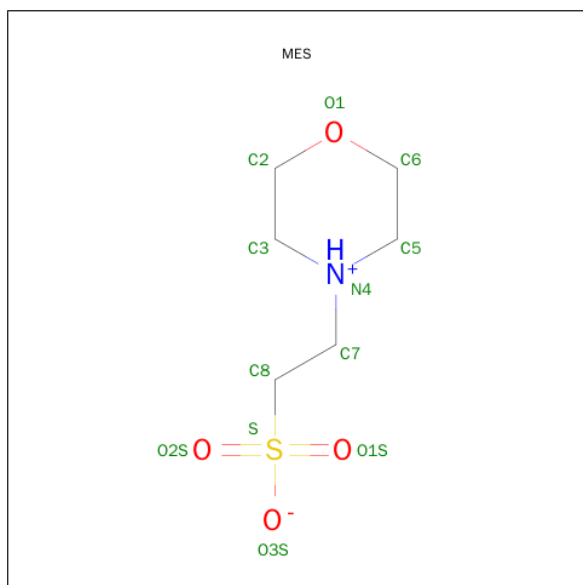
Chain	Residue	Modelled	Actual	Comment	Reference
D	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
D	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	310	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
E	615	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	1	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	32	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	150	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	201	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	293	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	310	MSE	MET	MODIFIED RESIDUE	UNP P31434

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Chain	Residue	Modelled	Actual	Comment	Reference
F	331	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	408	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	436	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	490	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	569	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	570	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	587	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	588	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	591	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	592	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	593	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	609	MSE	MET	MODIFIED RESIDUE	UNP P31434
F	615	MSE	MET	MODIFIED RESIDUE	UNP P31434

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

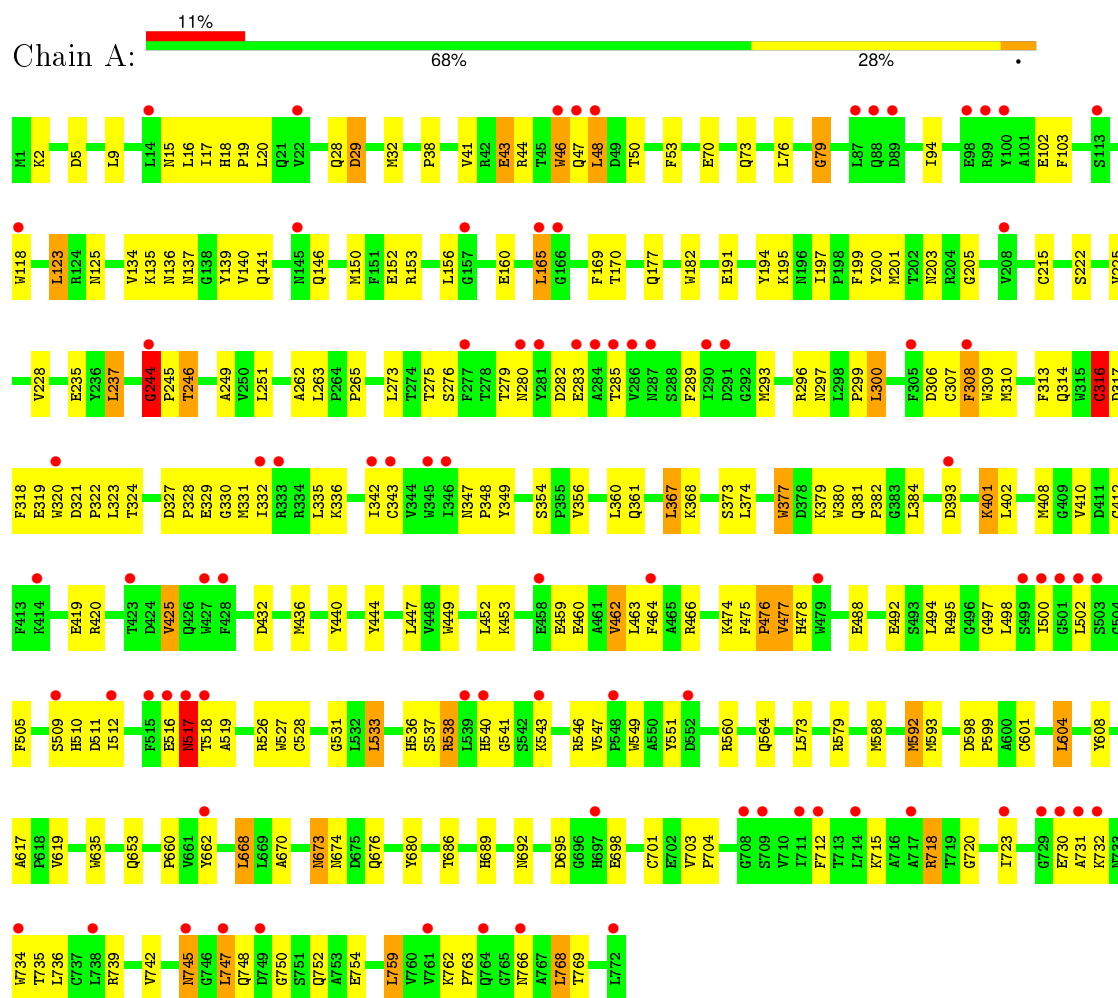
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	0
			86	86		
3	B	80	Total	O	0	0
			80	80		
3	C	108	Total	O	0	0
			108	108		
3	D	110	Total	O	0	0
			110	110		
3	E	61	Total	O	0	0
			61	61		
3	F	73	Total	O	0	0
			73	73		

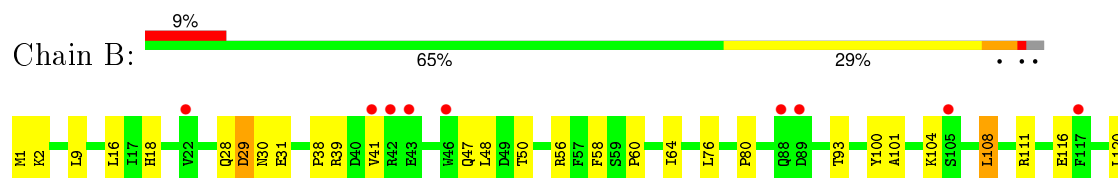
3 Residue-property plots

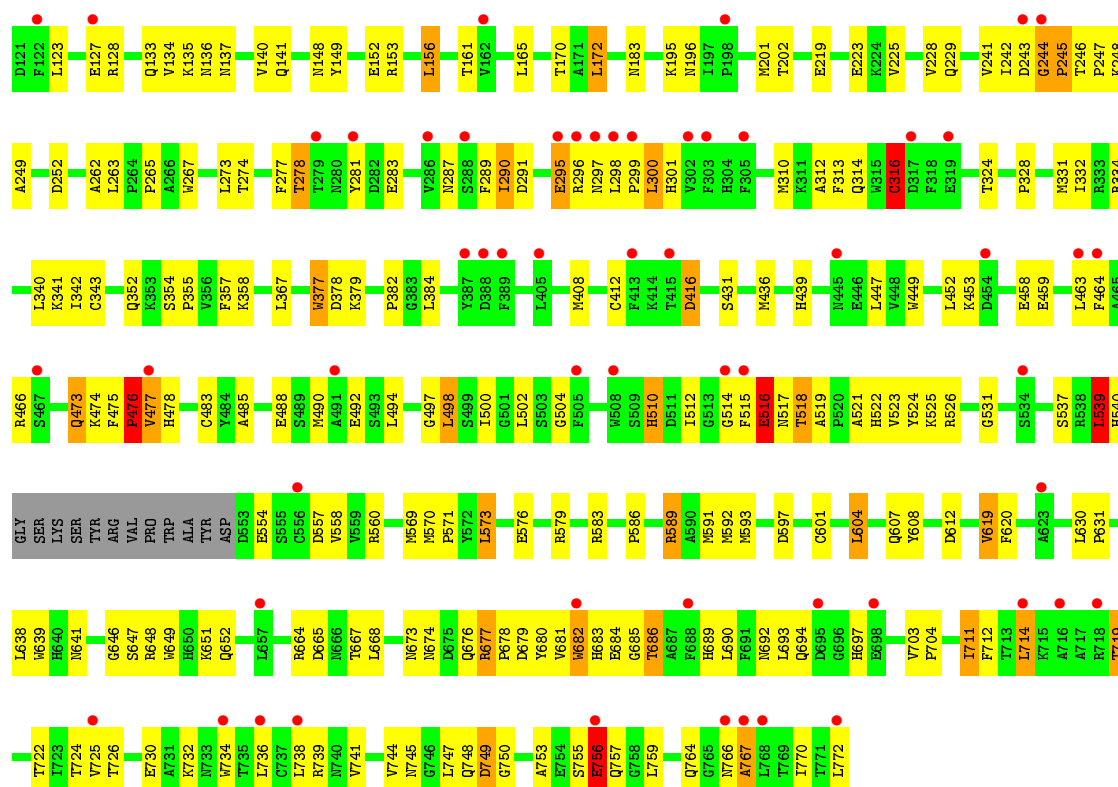
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

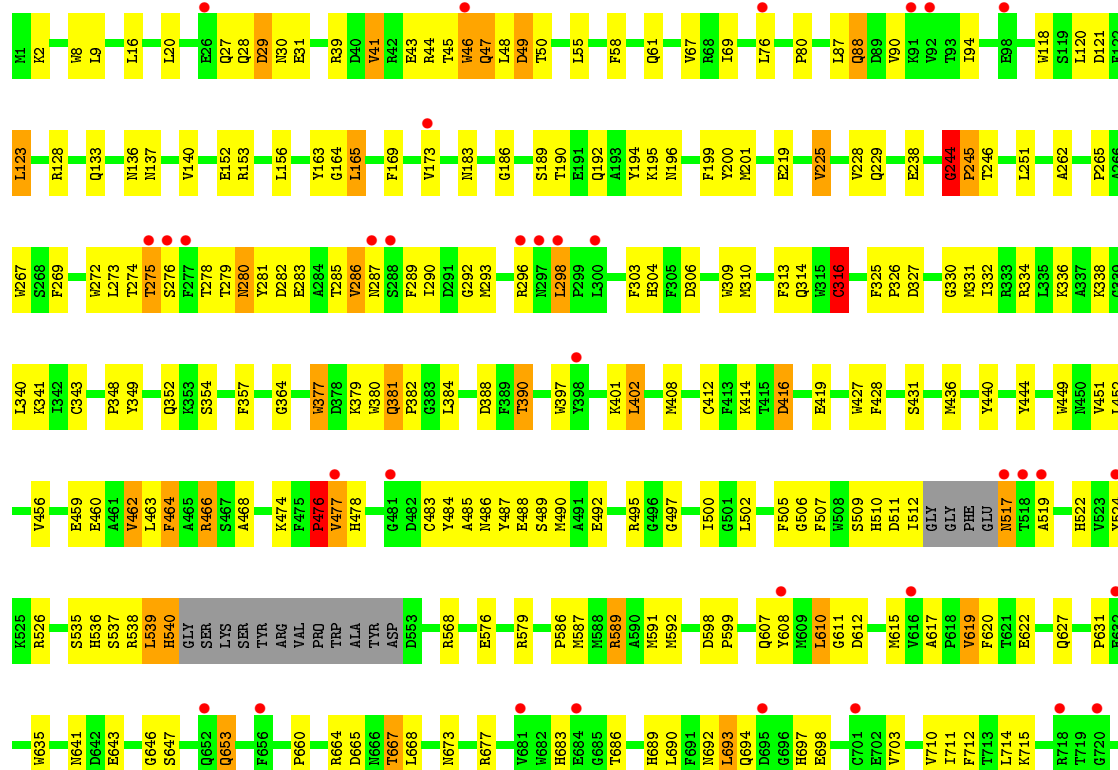


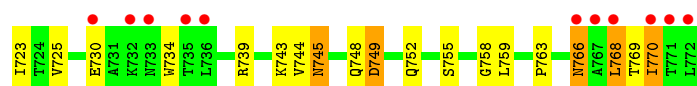
• Molecule 1: Putative family 31 glucosidase yicI



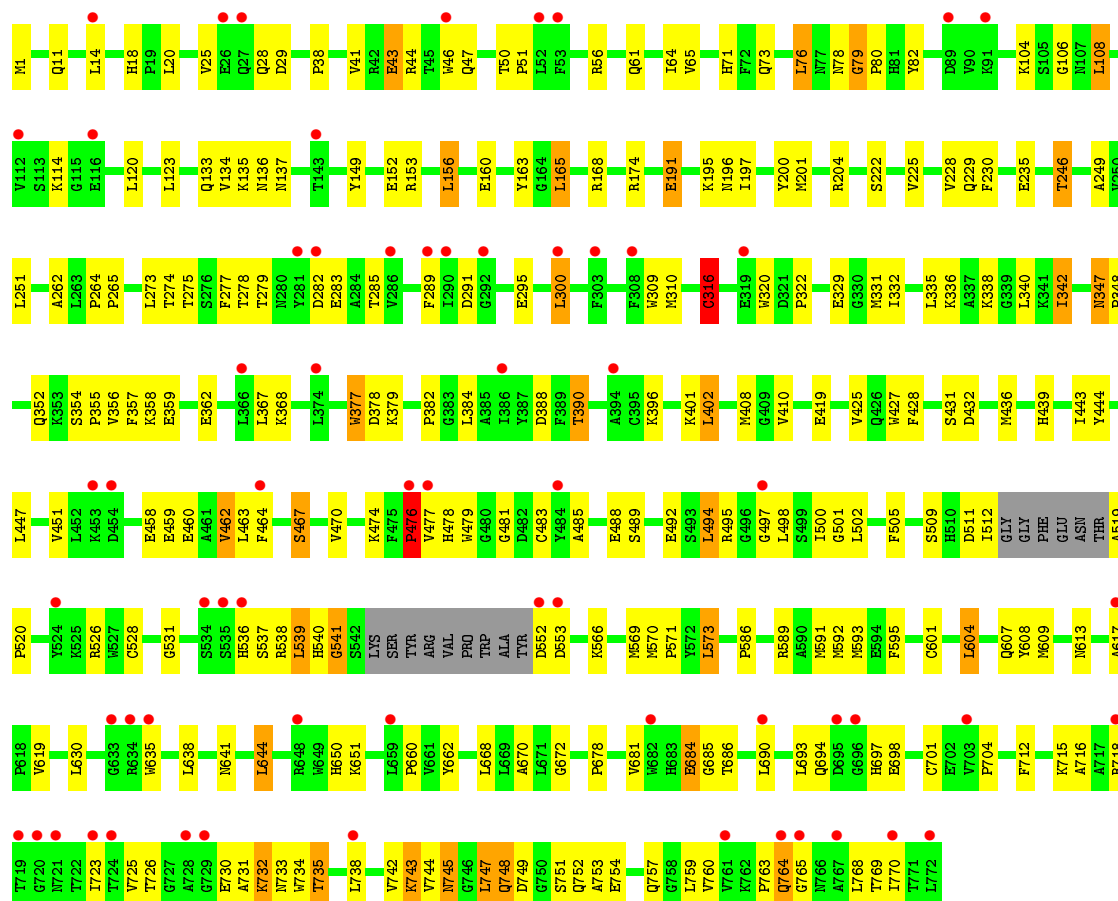


• Molecule 1: Putative family 31 glucosidase yici

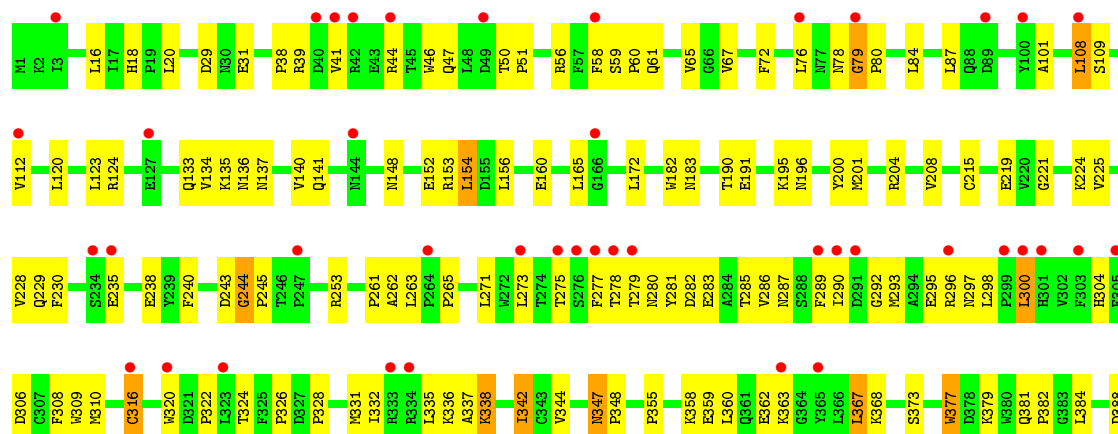


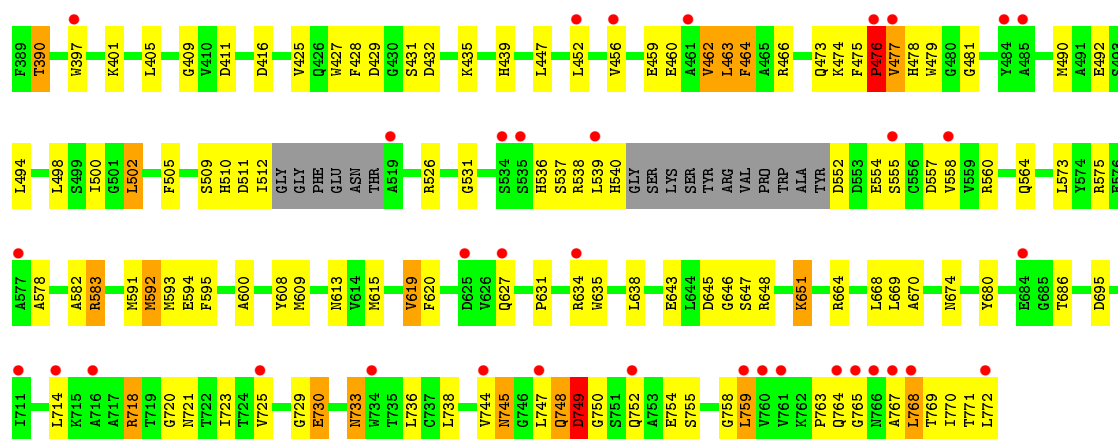


• Molecule 1: Putative family 31 glucosidase yicI

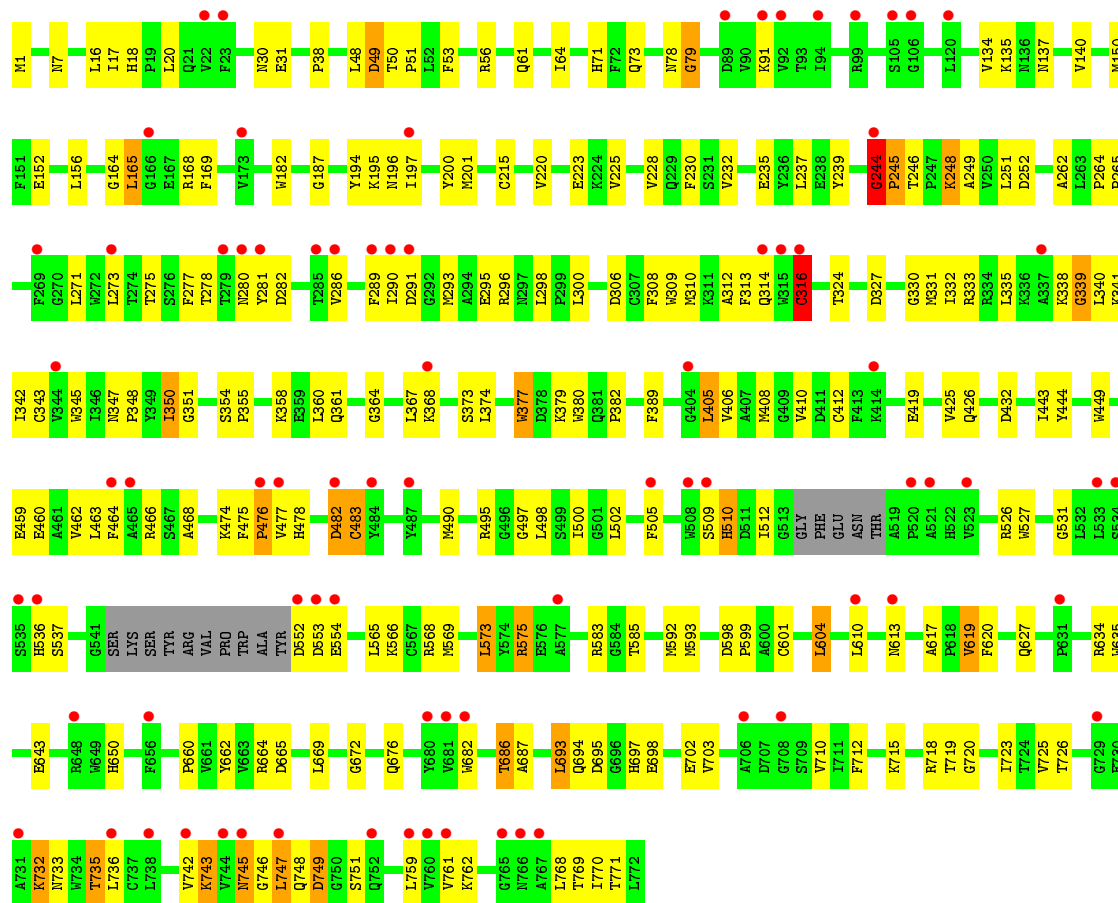


• Molecule 1: Putative family 31 glucosidase yicI





• 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	161.34Å 174.79Å 209.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 39.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (15.00-2.40) 99.2 (39.61-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.247 0.210 , 0.201	Depositor DCC
R_{free} test set	20672 reflections (9.07%)	DCC
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	5 of 228751 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	37302	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MES

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	0.38	0/6387	0.66	2/8650 (0.0%)
1	B	0.38	0/6280	0.66	4/8502 (0.0%)
1	C	0.40	0/6250	0.66	3/8461 (0.0%)
1	D	0.38	0/6253	0.66	3/8464 (0.0%)
1	E	0.38	0/6243	0.64	1/8451 (0.0%)
1	F	0.37	0/6251	0.64	1/8461 (0.0%)
All	All	0.38	0/37664	0.65	14/50989 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	CYS	CA-CB-SG	-6.30	102.66	114.00
1	C	316	CYS	CA-CB-SG	-6.12	102.99	114.00
1	C	416	ASP	N-CA-C	6.06	127.36	111.00
1	D	316	CYS	CA-CB-SG	-5.73	103.69	114.00
1	B	416	ASP	N-CA-C	5.69	126.36	111.00
1	F	244	GLY	N-CA-C	-5.51	99.34	113.10
1	D	279	THR	N-CA-C	5.44	125.69	111.00
1	A	244	GLY	N-CA-C	-5.41	99.58	113.10
1	D	613	ASN	N-CA-C	5.32	125.36	111.00
1	E	244	GLY	N-CA-C	-5.27	99.93	113.10
1	B	244	GLY	N-CA-C	-5.14	100.24	113.10
1	C	244	GLY	N-CA-C	-5.04	100.49	113.10
1	B	101	ALA	N-CA-C	-5.04	97.40	111.00
1	A	48	LEU	CA-CB-CG	5.04	126.88	115.30

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	6222	0	5932	236	0
1	B	6121	0	5839	225	0
1	C	6093	0	5817	231	0
1	D	6096	0	5816	202	0
1	E	6086	0	5808	230	0
1	F	6094	0	5814	192	0
2	A	12	0	13	1	0
2	B	12	0	13	0	0
2	C	12	0	13	2	0
2	D	12	0	13	0	0
2	E	12	0	13	1	0
2	F	12	0	13	0	0
3	A	86	0	0	1	0
3	B	80	0	0	3	0
3	C	108	0	0	3	0
3	D	110	0	0	2	0
3	E	61	0	0	1	0
3	F	73	0	0	1	0
All	All	37302	0	35104	1268	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1268) 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:E:591:MSE:SE	1:E:609:MSE:HE3	1.99	1.12
1:B:485:ALA:HB1	1:B:519:ALA:HB2	1.21	1.11
1:B:591:MSE:HE3	1:B:607:GLN:HG3	1.32	1.11
1:D:591:MSE:HE3	1:D:607:GLN:HG3	1.34	1.10
1:A:310:MSE:HE1	1:A:317:ASP:H	1.08	1.09
1:E:283:GLU:HA	1:E:331:MSE:HE3	1.33	1.07
1:A:32:MSE:HE2	1:A:94:ILE:HG23	1.21	1.07
1:B:358:LYS:HD2	1:B:358:LYS:H	1.08	1.06
1:B:690:LEU:HD11	1:B:693:LEU:HB2	1.31	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:CYS:HA	1:A:604:LEU:HD22	1.41	1.03
1:E:609:MSE:HE1	1:E:615:MSE:HG2	1.38	1.01
1:A:502:LEU:HD11	1:A:592:MSE:HE2	1.42	1.00
1:C:668:LEU:HD21	1:C:714:LEU:HD12	1.44	0.98
1:D:591:MSE:SE	1:D:609:MSE:HE2	2.15	0.96
1:B:379:LYS:HA	1:B:379:LYS:HE2	1.46	0.96
1:C:76:LEU:HD22	1:E:373:SER:HB3	1.49	0.94
1:A:246:THR:HG22	1:A:249:ALA:H	1.33	0.94
1:D:332:ILE:HD12	1:D:408:MSE:HE2	1.51	0.92
1:B:526:ARG:HD2	1:B:619:VAL:HG22	1.52	0.92
1:A:592:MSE:HE3	1:A:593:MSE:HB2	1.51	0.91
1:A:273:LEU:HB2	1:A:300:LEU:HD21	1.53	0.90
1:A:310:MSE:HE1	1:A:317:ASP:N	1.85	0.90
1:F:265:PRO:HD2	1:F:462:VAL:HG22	1.52	0.90
1:C:28:GLN:HA	1:C:28:GLN:HE21	1.36	0.90
1:B:358:LYS:N	1:B:358:LYS:HD2	1.86	0.89
1:E:609:MSE:HE1	1:E:615:MSE:CG	2.02	0.89
1:D:690:LEU:HD11	1:D:693:LEU:HB2	1.53	0.89
1:C:591:MSE:HE1	1:C:615:MSE:HG2	1.53	0.89
1:D:591:MSE:CE	1:D:607:GLN:HG3	2.05	0.87
1:B:589:ARG:HG2	1:B:593:MSE:CE	2.05	0.87
1:C:591:MSE:HE3	1:C:607:GLN:HE21	1.36	0.87
1:F:565:LEU:HG	1:F:569:MSE:HE2	1.54	0.87
1:B:485:ALA:CB	1:B:519:ALA:HB2	2.05	0.86
1:B:31:GLU:HG2	1:B:58:PHE:HB3	1.56	0.86
1:D:570:MSE:CE	1:D:573:LEU:HD23	2.06	0.85
1:F:443:ILE:HD12	1:F:444:TYR:N	1.92	0.85
1:F:526:ARG:HD2	1:F:619:VAL:HG22	1.58	0.84
1:F:332:ILE:HD12	1:F:408:MSE:HE2	1.58	0.84
1:D:283:GLU:HG3	1:D:331:MSE:HE3	1.58	0.84
1:B:358:LYS:H	1:B:358:LYS:CD	1.89	0.84
1:C:274:THR:HG22	1:C:304:HIS:HB3	1.57	0.84
1:B:641:ASN:ND2	1:B:757:GLN:HG3	1.93	0.83
1:A:275:THR:HG21	1:A:280:ASN:ND2	1.93	0.83
1:D:79:GLY:HA2	1:D:432:ASP:H	1.42	0.83
1:A:373:SER:HB3	1:E:76:LEU:HD22	1.60	0.83
1:D:519:ALA:HB3	1:D:520:PRO:HD3	1.61	0.83
1:B:668:LEU:HD13	1:B:690:LEU:HD23	1.60	0.83
1:A:332:ILE:HD12	1:A:408:MSE:HE2	1.59	0.83
1:D:246:THR:HG22	1:D:249:ALA:H	1.44	0.82
1:A:488:GLU:O	1:A:492:GLU:HG3	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:GLU:HA	1:E:331:MSE:CE	2.10	0.82
1:C:743:LYS:HA	1:C:759:LEU:HD12	1.62	0.82
1:D:11:GLN:HB2	1:D:14:LEU:HD22	1.59	0.81
1:B:589:ARG:HG2	1:B:593:MSE:HE1	1.60	0.81
1:E:609:MSE:CE	1:E:615:MSE:HG2	2.11	0.80
1:D:388:ASP:OD1	1:D:390:THR:HG22	1.81	0.80
1:E:526:ARG:HD2	1:E:619:VAL:HG22	1.62	0.80
1:E:609:MSE:HE1	1:E:615:MSE:CB	2.11	0.80
1:C:273:LEU:HD11	1:C:289:PHE:HE2	1.45	0.80
1:E:502:LEU:HD11	1:E:592:MSE:HE2	1.64	0.80
1:D:18:HIS:O	1:D:20:LEU:HD12	1.82	0.79
1:E:609:MSE:CE	1:E:615:MSE:HA	2.13	0.79
1:D:595:PHE:CE1	1:D:609:MSE:HE3	2.17	0.79
1:C:31:GLU:HG2	1:C:58:PHE:HB3	1.64	0.79
1:E:286:VAL:HG21	1:E:331:MSE:HE2	1.64	0.79
1:B:277:PHE:O	1:B:278:THR:HB	1.82	0.78
1:D:748:GLN:HB2	1:D:769:THR:HG22	1.66	0.77
1:A:763:PRO:HB3	1:A:768:LEU:HD12	1.66	0.77
1:A:32:MSE:HE2	1:A:94:ILE:CG2	2.10	0.77
1:E:282:ASP:O	1:E:285:THR:HG22	1.83	0.77
1:B:300:LEU:HD13	1:B:340:LEU:HD21	1.66	0.77
1:A:44:ARG:HH21	1:C:278:THR:HA	1.47	0.77
1:F:368:LYS:O	1:F:425:VAL:HG13	1.85	0.77
1:B:28:GLN:HG3	1:B:56:ARG:HH12	1.48	0.77
1:D:595:PHE:HE1	1:D:609:MSE:HE3	1.49	0.77
1:A:314:GLN:HB2	1:A:354:SER:HB2	1.66	0.77
1:B:591:MSE:CE	1:B:607:GLN:HG3	2.12	0.77
1:F:703:VAL:HG22	1:F:712:PHE:HB3	1.66	0.76
1:E:79:GLY:CA	1:E:432:ASP:H	1.99	0.76
1:E:755:SER:HB3	1:E:758:GLY:O	1.86	0.76
1:B:310:MSE:SE	1:B:316:CYS:HA	2.36	0.76
1:A:275:THR:HG21	1:A:280:ASN:HD21	1.49	0.76
1:A:518:THR:HG22	1:A:519:ALA:H	1.51	0.76
1:F:314:GLN:HB2	1:F:354:SER:HB2	1.67	0.76
1:C:44:ARG:O	1:C:47:GLN:HB2	1.86	0.76
1:E:342:ILE:HD13	1:E:342:ILE:H	1.51	0.76
1:E:767:ALA:O	1:E:768:LEU:HB2	1.84	0.75
1:E:695:ASP:HA	1:E:718:ARG:HD2	1.69	0.75
1:B:678:PRO:O	1:B:682:TRP:HZ3	1.70	0.75
1:B:287:ASN:HA	1:B:290:ILE:HG22	1.68	0.75
1:B:485:ALA:HB1	1:B:519:ALA:CB	2.10	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:GLU:HG2	1:E:58:PHE:HB3	1.67	0.75
1:A:170:THR:HG21	1:A:177:GLN:OE1	1.87	0.75
1:B:201:MSE:HE2	1:B:502:LEU:O	1.86	0.75
1:D:586:PRO:O	1:D:589:ARG:HD2	1.86	0.75
1:E:79:GLY:HA2	1:E:432:ASP:H	1.52	0.74
1:E:265:PRO:HG3	1:E:459:GLU:O	1.87	0.74
1:A:32:MSE:HE1	1:A:102:GLU:O	1.87	0.74
1:B:711:ILE:HD13	1:B:711:ILE:H	1.52	0.74
1:E:733:ASN:N	1:E:733:ASN:HD22	1.86	0.74
1:E:668:LEU:HD21	1:E:714:LEU:HD22	1.68	0.73
1:F:732:LYS:HA	1:F:732:LYS:HE2	1.68	0.73
1:B:474:LYS:C	1:B:476:PRO:HD3	2.08	0.73
1:D:262:ALA:HB3	1:D:476:PRO:HG2	1.69	0.73
1:C:269:PHE:HE2	1:C:587:MSE:HE1	1.54	0.73
1:F:195:LYS:HE2	1:F:478:HIS:HB3	1.69	0.73
1:A:313:PHE:HZ	1:E:41:VAL:HG21	1.54	0.73
1:B:677:ARG:HD3	1:B:679:ASP:O	1.89	0.73
1:C:310:MSE:SE	1:C:316:CYS:HA	2.39	0.73
1:A:283:GLU:HG3	1:A:331:MSE:HG3	1.72	0.72
1:C:332:ILE:HD12	1:C:408:MSE:HE2	1.70	0.72
1:F:300:LEU:HD22	1:F:340:LEU:HD21	1.69	0.72
1:E:310:MSE:SE	1:E:316:CYS:HA	2.40	0.72
1:F:566:LYS:HA	1:F:569:MSE:HE3	1.71	0.71
1:D:79:GLY:CA	1:D:432:ASP:H	2.02	0.71
1:C:539:LEU:O	1:C:540:HIS:HB2	1.90	0.71
1:A:262:ALA:HB3	1:A:476:PRO:HG2	1.72	0.71
1:E:108:LEU:HD23	1:E:109:SER:N	2.05	0.71
1:B:586:PRO:O	1:B:589:ARG:HD2	1.90	0.71
1:E:367:LEU:HD22	1:E:425:VAL:CG2	2.20	0.71
1:E:714:LEU:HD21	1:E:725:VAL:HG13	1.72	0.71
1:A:79:GLY:HA2	1:A:432:ASP:H	1.54	0.71
1:B:741:VAL:O	1:B:759:LEU:HB2	1.91	0.71
1:B:283:GLU:HG3	1:B:331:MSE:HG3	1.73	0.71
1:E:613:ASN:HB3	1:E:664:ARG:HG2	1.72	0.71
1:C:28:GLN:HA	1:C:28:GLN:NE2	2.06	0.71
1:A:703:VAL:HG22	1:A:712:PHE:HB3	1.73	0.70
1:B:689:HIS:CD2	1:B:739:ARG:HH11	2.09	0.70
1:D:368:LYS:O	1:D:425:VAL:HG22	1.91	0.70
1:D:570:MSE:HE2	1:D:573:LEU:HD23	1.72	0.70
1:C:703:VAL:CG1	1:C:712:PHE:HB3	2.21	0.70
1:B:772:LEU:H	1:B:772:LEU:HD22	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:THR:HG23	1:D:428:PHE:HB3	1.73	0.69
1:B:314:GLN:HB2	1:B:354:SER:HB2	1.73	0.69
1:A:273:LEU:HD21	1:A:289:PHE:HE1	1.57	0.69
1:C:591:MSE:HE3	1:C:607:GLN:NE2	2.06	0.69
1:D:367:LEU:HG	1:D:425:VAL:HG21	1.73	0.69
1:C:61:GLN:HB3	1:C:87:LEU:HD23	1.74	0.69
1:E:347:ASN:C	1:E:347:ASN:HD22	1.96	0.69
1:F:262:ALA:HB3	1:F:476:PRO:HG2	1.73	0.69
1:F:474:LYS:O	1:F:476:PRO:HD3	1.92	0.69
1:F:310:MSE:SE	1:F:316:CYS:HA	2.43	0.69
1:A:310:MSE:SE	1:A:316:CYS:HA	2.43	0.69
1:F:474:LYS:C	1:F:476:PRO:HD3	2.12	0.69
1:B:262:ALA:HB3	1:B:476:PRO:HG2	1.74	0.69
1:C:755:SER:HB3	1:C:758:GLY:O	1.93	0.69
1:C:88:GLN:H	1:C:88:GLN:CD	1.95	0.69
1:C:46:TRP:HA	1:C:46:TRP:CE3	2.27	0.69
1:E:295:GLU:O	1:E:296:ARG:HB2	1.93	0.68
1:A:592:MSE:HE3	1:A:593:MSE:CB	2.22	0.68
1:A:516:GLU:H	1:A:516:GLU:CD	1.97	0.68
1:D:526:ARG:HD2	1:D:619:VAL:HG22	1.75	0.68
1:C:262:ALA:HB3	1:C:476:PRO:HG2	1.75	0.68
1:A:279:THR:HG23	1:A:546:ARG:NH1	2.07	0.68
1:A:331:MSE:O	1:A:335:LEU:HD13	1.94	0.68
1:F:747:LEU:HD22	1:F:770:ILE:HG22	1.76	0.68
1:E:744:VAL:HG23	1:E:772:LEU:HA	1.75	0.68
1:F:725:VAL:HG13	1:F:768:LEU:HB3	1.76	0.68
1:D:291:ASP:O	1:D:295:GLU:HG3	1.94	0.68
1:D:512:ILE:CD1	1:D:531:GLY:HA3	2.24	0.68
1:B:100:TYR:CD2	1:B:111:ARG:HD3	2.29	0.68
1:E:609:MSE:HE2	1:E:615:MSE:HA	1.76	0.68
1:E:750:GLY:N	1:E:764:GLN:HG2	2.08	0.68
1:C:414:LYS:HD2	1:C:464:PHE:HB3	1.75	0.68
1:C:509:SER:HB3	1:C:536:HIS:HB2	1.74	0.68
1:F:425:VAL:CG1	1:F:426:GLN:N	2.57	0.68
1:B:703:VAL:O	1:B:711:ILE:HD13	1.93	0.68
1:D:698:GLU:OE2	1:D:715:LYS:HD3	1.93	0.68
1:F:265:PRO:HG3	1:F:459:GLU:O	1.94	0.68
1:B:571:PRO:HG3	1:B:682:TRP:HB2	1.76	0.67
1:E:44:ARG:HA	1:E:47:GLN:HG3	1.77	0.67
1:C:88:GLN:H	1:C:88:GLN:NE2	1.92	0.67
1:C:690:LEU:HD11	1:C:693:LEU:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:ASN:HD22	1:B:757:GLN:HG3	1.59	0.67
1:E:511:ASP:OD2	1:E:538:ARG:HD3	1.93	0.67
1:F:425:VAL:HG12	1:F:426:GLN:N	2.09	0.67
1:C:502:LEU:HD21	1:C:592:MSE:HE1	1.77	0.67
1:E:474:LYS:C	1:E:476:PRO:HD3	2.15	0.67
1:E:41:VAL:HG22	1:E:47:GLN:HG2	1.76	0.67
1:D:310:MSE:SE	1:D:316:CYS:HA	2.44	0.67
1:E:645:ASP:HB2	1:E:648:ARG:HH21	1.59	0.67
1:A:194:TYR:CD2	1:A:466:ARG:HD3	2.30	0.66
1:F:367:LEU:HD11	1:F:425:VAL:HG11	1.76	0.66
1:F:168:ARG:NH2	1:F:196:ASN:OD1	2.27	0.66
1:F:20:LEU:HD12	1:F:38:PRO:O	1.94	0.66
1:D:601:CYS:HA	1:D:604:LEU:HD22	1.78	0.66
1:E:627:GLN:HG2	1:E:651:LYS:HG2	1.77	0.66
1:B:690:LEU:CD1	1:B:693:LEU:HB2	2.20	0.66
1:D:474:LYS:C	1:D:476:PRO:HD3	2.15	0.66
1:B:474:LYS:O	1:B:476:PRO:HD3	1.95	0.66
1:D:748:GLN:CB	1:D:769:THR:HG22	2.25	0.66
1:D:195:LYS:HE2	1:D:478:HIS:HB3	1.77	0.66
1:C:169:PHE:O	1:F:225:VAL:HG11	1.96	0.66
1:D:591:MSE:HE1	1:D:608:TYR:N	2.11	0.66
1:A:512:ILE:HD11	1:A:531:GLY:HA3	1.78	0.66
1:C:27:GLN:HG3	1:C:94:ILE:HD12	1.78	0.66
1:D:694:GLN:HB2	1:D:697:HIS:CD2	2.30	0.66
1:E:367:LEU:HD22	1:E:425:VAL:HG21	1.78	0.65
1:A:79:GLY:CA	1:A:432:ASP:H	2.10	0.65
1:A:276:SER:HB3	1:A:279:THR:OG1	1.95	0.65
1:E:16:LEU:HD22	1:E:140:VAL:HG22	1.76	0.65
1:D:747:LEU:HD12	1:D:748:GLN:H	1.60	0.65
1:C:664:ARG:O	1:C:667:THR:HG23	1.96	0.65
1:C:698:GLU:OE2	1:C:715:LYS:HD3	1.96	0.65
1:B:281:TYR:O	1:B:324:THR:HG23	1.96	0.65
1:B:591:MSE:HE3	1:B:607:GLN:CG	2.19	0.65
1:F:761:VAL:HG11	1:F:768:LEU:HD21	1.79	0.65
1:A:768:LEU:HD13	1:A:768:LEU:H	1.61	0.65
1:F:367:LEU:CG	1:F:425:VAL:HG11	2.27	0.65
1:B:576:GLU:OE2	1:B:579:ARG:HD2	1.97	0.65
1:F:194:TYR:CD2	1:F:466:ARG:HD3	2.31	0.65
1:E:124:ARG:HD3	1:E:243:ASP:OD1	1.97	0.64
1:E:608:TYR:O	1:E:609:MSE:HE2	1.98	0.64
1:C:591:MSE:HE2	1:C:608:TYR:CA	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:PRO:HG3	1:B:682:TRP:CB	2.28	0.64
1:F:327:ASP:OD2	1:F:330:GLY:HA3	1.96	0.64
1:A:32:MSE:CE	1:A:94:ILE:HG23	2.12	0.64
1:F:137:ASN:HB3	1:F:152:GLU:OE1	1.95	0.64
1:B:463:LEU:O	1:B:477:VAL:HB	1.98	0.64
1:B:591:MSE:HE1	1:B:608:TYR:N	2.13	0.64
1:E:750:GLY:CA	1:E:764:GLN:HG2	2.28	0.64
1:B:382:PRO:HG3	1:D:50:THR:O	1.97	0.64
1:C:388:ASP:OD1	1:C:390:THR:HG22	1.98	0.64
1:E:331:MSE:O	1:E:335:LEU:HD23	1.97	0.64
1:C:46:TRP:HA	1:C:46:TRP:HE3	1.63	0.64
1:B:29:ASP:CG	1:B:30:ASN:H	2.01	0.64
1:A:474:LYS:C	1:A:476:PRO:HD3	2.18	0.63
1:D:483:CYS:HB3	1:D:489:SER:OG	1.98	0.63
1:D:137:ASN:HB3	1:D:152:GLU:OE1	1.97	0.63
1:A:310:MSE:CE	1:A:317:ASP:H	1.99	0.63
1:F:79:GLY:HA2	1:F:432:ASP:H	1.63	0.63
1:E:744:VAL:HG22	1:E:771:THR:O	1.99	0.63
1:E:592:MSE:HE3	1:E:593:MSE:HB2	1.80	0.63
1:C:16:LEU:HD22	1:C:140:VAL:HG22	1.81	0.62
1:A:463:LEU:O	1:A:477:VAL:HB	1.99	0.62
1:A:361:GLN:HG3	1:A:374:LEU:HD11	1.81	0.62
1:F:702:GLU:HB3	1:F:710:VAL:HG13	1.80	0.62
1:F:278:THR:HG22	1:F:308:PHE:CE1	2.34	0.62
1:E:763:PRO:HB2	1:E:765:GLY:O	1.98	0.62
1:C:522:HIS:CD2	1:C:622:GLU:HB2	2.35	0.62
1:A:310:MSE:CE	1:A:317:ASP:OD1	2.47	0.62
1:C:502:LEU:CD2	1:C:592:MSE:HE1	2.30	0.62
1:C:201:MSE:HE2	1:C:502:LEU:O	1.99	0.62
1:D:300:LEU:HD12	1:D:340:LEU:CD2	2.28	0.62
1:E:509:SER:HB3	1:E:536:HIS:HB2	1.82	0.62
1:B:16:LEU:HD22	1:B:140:VAL:HG22	1.81	0.62
1:A:201:MSE:CE	1:A:502:LEU:O	2.48	0.62
1:F:634:ARG:HD3	1:F:643:GLU:OE1	2.00	0.62
1:D:20:LEU:HD11	3:D:1129:HOH:O	1.99	0.61
1:C:27:GLN:HG3	1:C:94:ILE:CD1	2.30	0.61
1:B:377:TRP:CE2	1:B:379:LYS:HB2	2.35	0.61
1:C:273:LEU:HD11	1:C:289:PHE:CE2	2.30	0.61
1:E:31:GLU:OE1	1:E:56:ARG:HD3	2.00	0.61
1:D:474:LYS:O	1:D:476:PRO:HD3	1.99	0.61
1:E:609:MSE:HE1	1:E:615:MSE:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:693:LEU:HD13	1:F:718:ARG:HB2	1.81	0.61
1:B:297:ASN:C	1:B:299:PRO:HD3	2.20	0.61
1:A:509:SER:HB3	1:A:536:HIS:HB2	1.83	0.61
1:F:746:GLY:HA3	1:F:771:THR:OG1	2.00	0.61
1:D:511:ASP:OD1	1:D:538:ARG:HD2	2.00	0.61
1:F:48:LEU:HD12	1:F:49:ASP:HB2	1.81	0.61
1:F:296:ARG:O	1:F:298:LEU:HD13	2.01	0.61
1:F:150:MSE:HE3	1:F:235:GLU:C	2.20	0.61
1:C:586:PRO:O	1:C:589:ARG:HD2	2.00	0.61
1:C:507:PHE:HD2	1:C:587:MSE:HE2	1.65	0.61
1:E:560:ARG:O	1:E:564:GLN:HG3	2.01	0.61
1:D:354:SER:OG	1:D:356:VAL:HG12	2.00	0.61
1:C:456:VAL:HG12	1:C:460:GLU:CB	2.30	0.61
1:A:16:LEU:HD22	1:A:140:VAL:HG22	1.82	0.61
1:E:328:PRO:O	1:E:332:ILE:HD13	2.00	0.61
1:C:282:ASP:H	1:C:285:THR:CG2	2.13	0.61
1:B:711:ILE:HG12	1:B:712:PHE:N	2.15	0.61
1:E:733:ASN:N	1:E:733:ASN:ND2	2.49	0.61
1:C:41:VAL:HG22	1:C:47:GLN:HG3	1.81	0.60
1:C:507:PHE:CD2	1:C:587:MSE:HE2	2.36	0.60
1:E:368:LYS:O	1:E:425:VAL:HG22	2.01	0.60
1:C:484:TYR:HD2	1:C:486:ASN:ND2	1.99	0.60
1:C:269:PHE:CE2	1:C:587:MSE:HE1	2.36	0.60
1:B:539:LEU:O	1:B:540:HIS:HB3	2.01	0.60
1:B:290:ILE:HG13	1:B:340:LEU:HD11	1.83	0.60
1:F:703:VAL:CG2	1:F:712:PHE:HB3	2.30	0.60
1:E:390:THR:CG2	1:E:429:ASP:H	2.14	0.60
1:B:41:VAL:HG12	1:B:47:GLN:HG2	1.83	0.60
1:D:246:THR:CG2	1:D:249:ALA:H	2.14	0.60
1:C:474:LYS:C	1:C:476:PRO:HD3	2.22	0.60
1:B:638:LEU:HD12	1:B:639:TRP:HE3	1.66	0.60
1:A:32:MSE:HE1	1:A:102:GLU:C	2.22	0.60
1:B:641:ASN:HD22	1:B:757:GLN:CG	2.15	0.60
1:D:273:LEU:HD11	1:D:289:PHE:CE2	2.36	0.60
1:E:18:HIS:O	1:E:38:PRO:HA	2.01	0.60
1:C:283:GLU:HA	1:C:331:MSE:CE	2.30	0.60
1:E:609:MSE:HA	1:E:609:MSE:HE2	1.82	0.60
1:F:698:GLU:OE1	1:F:715:LYS:HD3	2.02	0.60
1:F:248:LYS:HD2	1:F:585:THR:HG23	1.82	0.60
1:C:61:GLN:HA	1:C:90:VAL:HG21	1.84	0.60
1:D:512:ILE:HD11	1:D:531:GLY:HA3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:694:GLN:HB2	1:C:697:HIS:CD2	2.37	0.60
1:B:497:GLY:O	1:B:500:ILE:HG22	2.02	0.60
1:A:41:VAL:HG22	1:A:47:GLN:HG2	1.83	0.60
1:A:205:GLY:O	1:A:244:GLY:O	2.20	0.60
1:E:342:ILE:HD11	1:E:409:GLY:O	2.02	0.60
1:C:485:ALA:HB1	1:C:519:ALA:CB	2.32	0.60
1:B:1:MSE:HE1	1:B:149:TYR:CZ	2.37	0.60
1:A:32:MSE:HE3	1:A:103:PHE:HB2	1.83	0.59
1:B:744:VAL:HG13	1:B:772:LEU:HA	1.84	0.59
1:A:511:ASP:OD1	1:A:540:HIS:HD2	1.85	0.59
1:E:738:LEU:HD22	1:E:738:LEU:H	1.66	0.59
1:A:246:THR:HG22	1:A:249:ALA:N	2.12	0.59
1:B:300:LEU:CD1	1:B:340:LEU:HD21	2.32	0.59
1:E:72:PHE:H	1:E:235:GLU:HG3	1.66	0.59
1:C:123:LEU:HD22	1:C:123:LEU:N	2.16	0.59
1:F:361:GLN:HG3	1:F:374:LEU:HD11	1.83	0.59
1:D:274:THR:O	1:D:541:GLY:N	2.35	0.59
1:A:150:MSE:HE3	1:A:235:GLU:C	2.22	0.59
1:D:342:ILE:HD11	1:D:410:VAL:HG22	1.85	0.59
1:C:591:MSE:HE2	1:C:608:TYR:N	2.17	0.59
1:E:750:GLY:HA2	1:E:764:GLN:HG2	1.83	0.59
1:C:698:GLU:CD	1:C:715:LYS:HD3	2.23	0.59
1:E:273:LEU:HD22	1:E:300:LEU:HD21	1.84	0.59
1:D:591:MSE:HE3	1:D:607:GLN:CG	2.21	0.59
1:C:485:ALA:HB1	1:C:519:ALA:HB2	1.84	0.59
1:C:244:GLY:O	1:C:245:PRO:C	2.40	0.59
1:A:731:ALA:C	1:A:732:LYS:HD2	2.22	0.59
1:A:689:HIS:CD2	1:A:739:ARG:HH11	2.21	0.59
1:B:591:MSE:HE1	1:B:608:TYR:CA	2.33	0.59
1:C:743:LYS:NZ	1:C:743:LYS:HB3	2.18	0.59
1:F:350:ILE:HD13	1:F:351:GLY:O	2.02	0.59
1:F:509:SER:HB3	1:F:536:HIS:HB2	1.85	0.59
1:E:283:GLU:CA	1:E:331:MSE:HE3	2.19	0.59
1:A:297:ASN:O	1:A:299:PRO:HD3	2.02	0.59
1:B:601:CYS:HA	1:B:604:LEU:HD22	1.85	0.59
1:F:265:PRO:CD	1:F:462:VAL:HG22	2.30	0.59
1:A:518:THR:HG22	1:A:519:ALA:N	2.17	0.59
1:B:328:PRO:CB	1:B:408:MSE:HE1	2.33	0.59
1:C:744:VAL:HG11	1:C:770:ILE:HD11	1.83	0.59
1:C:290:ILE:HD11	1:C:338:LYS:HD2	1.84	0.59
1:E:748:GLN:HG3	1:E:769:THR:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:HG13	1:D:495:ARG:NH2	2.17	0.58
1:C:631:PRO:O	1:C:646:GLY:HA3	2.02	0.58
1:F:367:LEU:CD1	1:F:425:VAL:HG11	2.32	0.58
1:F:500:ILE:HG12	1:F:505:PHE:HB2	1.85	0.58
1:E:609:MSE:HE1	1:E:615:MSE:CA	2.33	0.58
1:C:332:ILE:CD1	1:C:408:MSE:HE2	2.32	0.58
1:B:111:ARG:HD2	3:B:1450:HOH:O	2.02	0.58
1:F:79:GLY:CA	1:F:432:ASP:H	2.15	0.58
1:F:296:ARG:HH12	1:F:553:ASP:CG	2.07	0.58
1:A:244:GLY:O	1:A:245:PRO:C	2.42	0.58
1:A:273:LEU:CB	1:A:300:LEU:HD21	2.30	0.58
1:B:290:ILE:HD13	1:B:290:ILE:O	2.03	0.58
1:B:576:GLU:HA	1:B:579:ARG:HG3	1.86	0.58
1:A:169:PHE:O	1:D:225:VAL:HG11	2.04	0.58
1:D:749:ASP:O	1:D:764:GLN:HG3	2.03	0.58
1:F:350:ILE:HD11	1:F:354:SER:HB3	1.85	0.58
1:C:283:GLU:O	1:C:287:ASN:HB2	2.03	0.58
1:B:674:ASN:HB3	1:B:680:TYR:CE1	2.37	0.58
1:B:41:VAL:HG12	1:B:41:VAL:O	2.03	0.58
1:F:497:GLY:O	1:F:500:ILE:HG22	2.03	0.58
1:A:718:ARG:HB2	1:A:723:ILE:HG12	1.85	0.58
1:E:72:PHE:HB2	1:E:235:GLU:CG	2.33	0.58
1:B:517:ASN:O	1:B:518:THR:HG23	2.04	0.58
1:E:464:PHE:HE2	1:E:538:ARG:HD2	1.69	0.58
1:F:18:HIS:O	1:F:38:PRO:HA	2.02	0.58
1:C:589:ARG:NH2	1:C:612:ASP:OD2	2.33	0.58
1:A:419:GLU:OE2	1:A:466:ARG:HD2	2.04	0.57
1:C:495:ARG:NH2	1:F:225:VAL:CG1	2.66	0.57
1:B:750:GLY:N	1:B:764:GLN:HG2	2.19	0.57
1:A:332:ILE:HD12	1:A:408:MSE:CE	2.31	0.57
1:F:732:LYS:CE	1:F:733:ASN:H	2.16	0.57
1:E:244:GLY:HA2	1:E:253:ARG:HH12	1.69	0.57
1:A:732:LYS:HD2	1:A:732:LYS:N	2.19	0.57
1:A:293:MSE:HE2	1:A:549:TRP:CH2	2.39	0.57
1:C:380:TRP:CH2	2:C:803:MES:H21	2.39	0.57
1:D:153:ARG:HG2	1:D:229:GLN:HB2	1.86	0.57
1:C:766:ASN:C	1:C:766:ASN:HD22	2.08	0.57
1:D:358:LYS:O	1:D:362:GLU:HG3	2.05	0.57
1:A:601:CYS:HA	1:A:604:LEU:CD2	2.26	0.57
1:D:763:PRO:HB3	1:D:768:LEU:HD11	1.86	0.57
1:C:265:PRO:CD	1:C:462:VAL:HG22	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:752:GLN:HG3	1:D:759:LEU:HD11	1.86	0.57
1:A:43:GLU:HG2	1:A:46:TRP:HB2	1.86	0.57
1:B:631:PRO:O	1:B:646:GLY:HA3	2.05	0.57
1:E:613:ASN:HD22	1:E:664:ARG:HD3	1.69	0.57
1:D:300:LEU:HD12	1:D:340:LEU:HD22	1.86	0.57
1:F:273:LEU:HD11	1:F:289:PHE:CE1	2.39	0.57
1:B:352:GLN:NE2	1:D:73:GLN:HG3	2.19	0.57
1:A:273:LEU:HD21	1:A:289:PHE:CE1	2.39	0.57
1:E:347:ASN:ND2	1:E:347:ASN:C	2.58	0.57
1:A:730:GLU:OE2	1:A:732:LYS:HE3	2.03	0.57
1:C:275:THR:HG21	1:C:280:ASN:HB3	1.86	0.57
1:F:237:LEU:CD1	1:F:239:TYR:HD2	2.17	0.57
1:E:265:PRO:HD2	1:E:462:VAL:HG22	1.85	0.57
1:A:474:LYS:O	1:A:476:PRO:HD3	2.05	0.57
1:E:273:LEU:HB3	1:E:300:LEU:HD11	1.86	0.57
1:E:463:LEU:O	1:E:477:VAL:HB	2.05	0.57
1:B:379:LYS:HA	1:B:379:LYS:CE	2.29	0.57
1:C:535:SER:HA	1:C:587:MSE:HE3	1.86	0.57
1:C:495:ARG:HH21	1:F:225:VAL:CG1	2.18	0.57
1:E:243:ASP:CG	1:E:244:GLY:H	2.07	0.57
1:E:324:THR:O	1:E:326:PRO:HD3	2.05	0.57
1:A:123:LEU:HD22	1:A:123:LEU:N	2.19	0.57
1:E:123:LEU:HD22	1:E:123:LEU:N	2.20	0.57
1:A:698:GLU:CD	1:A:715:LYS:HE2	2.25	0.57
1:A:516:GLU:HB3	1:A:543:LYS:NZ	2.20	0.57
1:E:72:PHE:HB2	1:E:235:GLU:HG2	1.85	0.57
1:D:509:SER:HB3	1:D:536:HIS:HB2	1.86	0.56
1:E:747:LEU:HD23	1:E:748:GLN:N	2.21	0.56
1:E:367:LEU:HD22	1:E:425:VAL:HG22	1.86	0.56
1:F:768:LEU:HD12	1:F:769:THR:H	1.69	0.56
1:A:150:MSE:HG2	1:A:237:LEU:HB2	1.88	0.56
1:A:343:CYS:HB2	1:A:412:CYS:SG	2.45	0.56
1:B:265:PRO:HG3	1:B:459:GLU:O	2.05	0.56
1:C:748:GLN:HB3	1:C:769:THR:CG2	2.35	0.56
1:C:48:LEU:HD12	1:C:49:ASP:HB2	1.86	0.56
1:A:494:LEU:HD12	1:A:588:MSE:HE3	1.87	0.56
1:D:28:GLN:HG3	1:D:56:ARG:HH12	1.69	0.56
1:B:554:GLU:O	1:B:558:VAL:HG23	2.06	0.56
1:B:301:HIS:HE2	1:B:677:ARG:HA	1.70	0.56
1:D:347:ASN:C	1:D:347:ASN:HD22	2.08	0.56
1:F:348:PRO:HD3	1:F:444:TYR:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:531:GLY:O	1:F:537:SER:HB3	2.05	0.56
1:D:571:PRO:HB2	1:D:670:ALA:O	2.06	0.56
1:E:195:LYS:HE2	1:E:478:HIS:HB3	1.87	0.56
1:C:8:TRP:C	1:C:9:LEU:HD12	2.26	0.56
1:F:347:ASN:HB2	1:F:348:PRO:HD2	1.88	0.56
1:F:443:ILE:HD12	1:F:444:TYR:H	1.70	0.56
1:E:287:ASN:O	1:E:290:ILE:HG12	2.06	0.56
1:D:690:LEU:HD11	1:D:693:LEU:CB	2.33	0.56
1:E:368:LYS:O	1:E:425:VAL:CG2	2.54	0.56
1:A:689:HIS:HD2	1:A:739:ARG:HD3	1.71	0.56
1:A:46:TRP:HA	1:A:46:TRP:HE3	1.71	0.56
1:A:265:PRO:CD	1:A:462:VAL:HG22	2.36	0.56
1:B:195:LYS:HE2	1:B:478:HIS:HB3	1.87	0.56
1:D:329:GLU:N	1:D:408:MSE:HE3	2.22	0.55
1:B:447:LEU:C	1:B:447:LEU:HD23	2.26	0.55
1:E:512:ILE:CD1	1:E:531:GLY:HA3	2.35	0.55
1:F:482:ASP:O	1:F:483:CYS:HB2	2.06	0.55
1:D:282:ASP:OD1	1:D:285:THR:HG23	2.06	0.55
1:A:16:LEU:CD2	1:A:140:VAL:HG22	2.36	0.55
1:A:367:LEU:HD21	1:A:425:VAL:CG1	2.36	0.55
1:D:265:PRO:HG3	1:D:460:GLU:HA	1.87	0.55
1:E:295:GLU:C	1:E:297:ASN:H	2.08	0.55
1:B:352:GLN:HA	1:B:357:PHE:CD1	2.42	0.55
1:A:367:LEU:HD22	1:A:425:VAL:HG22	1.89	0.55
1:E:381:GLN:HB2	1:E:384:LEU:HD12	1.88	0.55
1:C:526:ARG:HD2	1:C:619:VAL:HG22	1.89	0.55
1:C:279:THR:O	1:C:281:TYR:N	2.39	0.55
1:F:715:LYS:O	1:F:725:VAL:HA	2.07	0.55
1:A:367:LEU:HD22	1:A:425:VAL:CG2	2.37	0.55
1:A:592:MSE:HE3	1:A:593:MSE:CA	2.37	0.55
1:D:485:ALA:HB1	1:D:519:ALA:N	2.21	0.55
1:A:41:VAL:HG21	1:C:313:PHE:HZ	1.72	0.55
1:A:698:GLU:OE2	1:A:715:LYS:HE2	2.06	0.55
1:D:133:GLN:O	1:D:136:ASN:HB2	2.06	0.55
1:A:146:GLN:HA	1:A:146:GLN:HE21	1.71	0.55
1:C:703:VAL:HG12	1:C:712:PHE:HB3	1.87	0.55
1:E:342:ILE:HD13	1:E:342:ILE:N	2.20	0.55
1:B:244:GLY:O	1:B:246:THR:N	2.40	0.55
1:E:200:TYR:CE2	1:E:228:VAL:HG11	2.42	0.55
1:C:591:MSE:CE	1:C:607:GLN:HE21	2.16	0.55
1:E:265:PRO:CD	1:E:462:VAL:HG22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:LEU:HD11	1:D:289:PHE:HE2	1.71	0.55
1:A:46:TRP:HA	1:A:46:TRP:CE3	2.41	0.55
1:D:165:LEU:HD13	1:D:200:TYR:HB3	1.88	0.55
1:A:195:LYS:NZ	1:A:478:HIS:HB3	2.21	0.55
1:E:134:VAL:O	1:E:135:LYS:HB2	2.06	0.55
1:A:246:THR:HG23	3:A:1042:HOH:O	2.07	0.54
1:B:248:LYS:HG3	1:B:593:MSE:HE3	1.89	0.54
1:E:342:ILE:HD13	1:E:411:ASP:OD1	2.07	0.54
1:B:328:PRO:HB3	1:B:408:MSE:HE1	1.89	0.54
1:B:136:ASN:HB3	1:B:153:ARG:HB2	1.90	0.54
1:A:170:THR:CG2	1:A:177:GLN:OE1	2.56	0.54
1:C:67:VAL:O	1:C:238:GLU:HA	2.07	0.54
1:A:18:HIS:O	1:A:38:PRO:HA	2.08	0.54
1:B:591:MSE:HG2	1:B:604:LEU:HD23	1.90	0.54
1:E:286:VAL:CG2	1:E:331:MSE:HE2	2.36	0.54
1:B:28:GLN:HG3	1:B:56:ARG:NH1	2.22	0.54
1:B:108:LEU:HG	1:B:243:ASP:HB2	1.90	0.54
1:E:39:ARG:HH22	1:E:46:TRP:HB3	1.72	0.54
1:D:168:ARG:HB2	1:D:174:ARG:NH1	2.23	0.54
1:D:591:MSE:HE1	1:D:608:TYR:CA	2.37	0.54
1:E:464:PHE:CE2	1:E:538:ARG:HD2	2.43	0.54
1:B:483:CYS:O	1:B:514:GLY:HA2	2.08	0.54
1:D:71:HIS:HD2	1:D:235:GLU:OE1	1.91	0.54
1:D:742:VAL:HG23	1:D:743:LYS:H	1.73	0.54
1:A:617:ALA:HB3	1:A:660:PRO:HB2	1.89	0.54
1:F:379:LYS:HA	1:F:379:LYS:HE2	1.90	0.54
1:D:390:THR:CG2	1:D:428:PHE:HB3	2.37	0.54
1:A:265:PRO:HG3	1:A:460:GLU:HA	1.90	0.54
1:A:377:TRP:CE2	1:A:379:LYS:HB2	2.43	0.54
1:E:152:GLU:HB3	1:E:230:PHE:CE1	2.43	0.54
1:F:306:ASP:O	1:F:309:TRP:HD1	1.91	0.54
1:E:320:TRP:O	1:E:322:PRO:HD3	2.08	0.54
1:C:745:ASN:C	1:C:745:ASN:HD22	2.11	0.54
1:A:748:GLN:O	1:A:768:LEU:HB2	2.07	0.54
1:B:287:ASN:HA	1:B:290:ILE:CG2	2.38	0.54
1:B:512:ILE:HD12	1:B:539:LEU:HA	1.90	0.54
1:A:495:ARG:NH2	1:D:225:VAL:CG1	2.71	0.54
1:B:50:THR:O	1:F:382:PRO:HG3	2.07	0.54
1:F:367:LEU:HG	1:F:425:VAL:HG11	1.89	0.53
1:A:146:GLN:HA	1:A:146:GLN:NE2	2.23	0.53
1:B:343:CYS:HB2	1:B:412:CYS:SG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:575:ARG:HG3	1:F:702:GLU:O	2.09	0.53
1:E:38:PRO:HG3	1:E:51:PRO:HD2	1.90	0.53
1:D:61:GLN:HB2	1:D:64:ILE:HD12	1.90	0.53
1:F:291:ASP:O	1:F:295:GLU:HG3	2.09	0.53
1:C:511:ASP:OD1	1:C:538:ARG:HD2	2.08	0.53
1:E:490:MSE:HE2	1:E:620:PHE:CE2	2.43	0.53
1:A:279:THR:O	1:A:279:THR:HG22	2.08	0.53
1:D:20:LEU:HD13	1:D:38:PRO:C	2.28	0.53
1:C:456:VAL:HG12	1:C:460:GLU:HB2	1.91	0.53
1:F:389:PHE:HB2	1:F:443:ILE:HD13	1.90	0.53
1:C:41:VAL:HG13	1:C:41:VAL:O	2.07	0.53
1:E:768:LEU:HD23	1:E:769:THR:N	2.24	0.53
1:A:516:GLU:HB3	1:A:543:LYS:HZ2	1.72	0.53
1:E:273:LEU:HD21	1:E:289:PHE:CE1	2.44	0.53
1:A:327:ASP:OD2	1:A:330:GLY:HA3	2.07	0.53
1:E:752:GLN:HB2	1:E:759:LEU:HD11	1.89	0.53
1:D:723:ILE:HB	1:D:770:ILE:HB	1.90	0.53
1:A:283:GLU:HG3	1:A:331:MSE:CG	2.39	0.53
1:B:283:GLU:HG3	1:B:331:MSE:CG	2.39	0.53
1:D:265:PRO:HD2	1:D:462:VAL:HG22	1.90	0.53
1:B:473:GLN:HG2	1:B:504:GLY:O	2.09	0.53
1:F:694:GLN:HB2	1:F:697:HIS:CD2	2.44	0.53
1:F:601:CYS:HA	1:F:604:LEU:HD22	1.90	0.53
1:A:222:SER:O	1:D:191:GLU:HG2	2.08	0.53
1:D:715:LYS:HB3	1:D:726:THR:HG22	1.89	0.53
1:C:282:ASP:H	1:C:285:THR:HG22	1.72	0.53
1:F:723:ILE:HB	1:F:770:ILE:HG13	1.90	0.53
1:E:390:THR:HG22	1:E:428:PHE:HB3	1.91	0.53
1:E:390:THR:HG21	1:E:427:TRP:HB3	1.89	0.53
1:F:31:GLU:OE2	1:F:56:ARG:HD3	2.09	0.53
1:A:668:LEU:HB3	1:A:701:CYS:HB2	1.91	0.53
1:F:246:THR:HG23	1:F:249:ALA:H	1.73	0.53
1:F:244:GLY:O	1:F:246:THR:N	2.42	0.53
1:D:566:LYS:HG2	1:D:570:MSE:HE3	1.91	0.53
1:A:511:ASP:OD2	1:A:538:ARG:HD2	2.09	0.53
1:B:246:THR:HG23	1:B:249:ALA:H	1.73	0.53
1:A:20:LEU:HD22	1:A:134:VAL:HG22	1.90	0.53
1:D:497:GLY:O	1:D:500:ILE:HG22	2.09	0.53
1:C:743:LYS:HA	1:C:759:LEU:CD1	2.38	0.52
1:B:719:THR:O	1:B:722:THR:HG22	2.09	0.52
1:D:617:ALA:O	1:D:660:PRO:HD2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:MSE:HE2	1:E:502:LEU:O	2.08	0.52
1:B:744:VAL:HG12	1:B:745:ASN:N	2.24	0.52
1:C:397:TRP:CZ2	1:C:401:LYS:HE3	2.43	0.52
1:D:332:ILE:O	1:D:336:LYS:HG3	2.10	0.52
1:F:187:GLY:HA2	1:F:482:ASP:OD2	2.09	0.52
1:B:714:LEU:HD21	1:B:725:VAL:CG1	2.40	0.52
1:F:310:MSE:SE	1:F:316:CYS:H	2.42	0.52
1:F:748:GLN:O	1:F:749:ASP:HB2	2.09	0.52
1:E:730:GLU:HG3	1:E:730:GLU:O	2.09	0.52
1:B:244:GLY:O	1:B:245:PRO:C	2.46	0.52
1:B:747:LEU:HD13	1:B:770:ILE:HG12	1.91	0.52
1:D:273:LEU:HB2	1:D:300:LEU:HD21	1.91	0.52
1:D:763:PRO:HB3	1:D:768:LEU:CD1	2.40	0.52
1:E:594:GLU:HG3	1:E:609:MSE:HG3	1.90	0.52
1:D:283:GLU:HA	1:D:331:MSE:CE	2.40	0.52
1:E:595:PHE:CE1	1:E:631:PRO:HG2	2.45	0.52
1:E:359:GLU:O	1:E:363:LYS:HG2	2.08	0.52
1:C:352:GLN:HA	1:C:357:PHE:CD1	2.45	0.52
1:B:449:TRP:CH2	1:B:476:PRO:HD2	2.45	0.52
1:C:283:GLU:HA	1:C:331:MSE:HE3	1.91	0.52
1:A:150:MSE:CG	1:A:237:LEU:HB2	2.40	0.52
1:D:348:PRO:HD3	1:D:444:TYR:CZ	2.45	0.52
1:D:160:GLU:HG3	1:D:204:ARG:HG2	1.92	0.52
1:B:80:PRO:HD3	1:B:436:MSE:HE2	1.91	0.52
1:C:195:LYS:HE2	1:C:478:HIS:HB3	1.92	0.52
1:A:310:MSE:SE	1:A:316:CYS:H	2.42	0.51
1:B:589:ARG:NH2	1:B:612:ASP:OD1	2.41	0.51
1:B:689:HIS:HD2	1:B:739:ARG:HD3	1.75	0.51
1:B:133:GLN:HB2	1:B:136:ASN:HD22	1.75	0.51
1:F:343:CYS:HB2	1:F:412:CYS:SG	2.50	0.51
1:C:377:TRP:CE2	1:C:379:LYS:HB2	2.44	0.51
1:B:673:ASN:ND2	1:B:684:GLU:O	2.43	0.51
1:E:502:LEU:HD11	1:E:592:MSE:CE	2.37	0.51
1:C:390:THR:CG2	1:C:428:PHE:HB3	2.41	0.51
1:C:225:VAL:CG1	1:F:495:ARG:NH2	2.74	0.51
1:C:190:THR:HA	1:F:223:GLU:O	2.10	0.51
1:D:651:LYS:C	1:D:651:LYS:HD3	2.30	0.51
1:C:50:THR:O	1:E:382:PRO:HG3	2.10	0.51
1:D:569:MSE:HB3	1:D:573:LEU:HD22	1.91	0.51
1:C:539:LEU:O	1:C:540:HIS:CB	2.58	0.51
1:C:711:ILE:HG12	1:C:711:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:MSE:CE	1:D:502:LEU:O	2.59	0.51
1:B:267:TRP:CE3	1:B:341:LYS:HG3	2.45	0.51
1:A:560:ARG:O	1:A:564:GLN:HG3	2.09	0.51
1:F:338:LYS:HD3	1:F:339:GLY:N	2.26	0.51
1:A:265:PRO:HD2	1:A:462:VAL:HG22	1.93	0.51
1:D:352:GLN:HA	1:D:357:PHE:CD1	2.45	0.51
1:C:535:SER:CB	1:C:587:MSE:HE3	2.40	0.51
1:E:20:LEU:HD12	1:E:38:PRO:O	2.11	0.51
1:A:70:GLU:OE2	1:A:73:GLN:NE2	2.31	0.51
1:B:225:VAL:HG11	1:E:492:GLU:HG2	1.92	0.51
1:B:170:THR:HG22	1:E:225:VAL:HG12	1.92	0.51
1:B:299:PRO:HG2	1:B:676:GLN:OE1	2.11	0.51
1:F:71:HIS:HD2	1:F:235:GLU:OE1	1.94	0.51
1:A:382:PRO:HG3	1:E:50:THR:O	2.11	0.51
1:E:401:LYS:O	1:E:405:LEU:HD13	2.11	0.51
1:F:617:ALA:HB3	1:F:660:PRO:HB2	1.92	0.51
1:B:526:ARG:HD2	1:B:619:VAL:CG2	2.33	0.51
1:F:195:LYS:HB3	1:F:468:ALA:HB3	1.91	0.51
1:E:645:ASP:HB2	1:E:648:ARG:NH2	2.25	0.51
1:B:522:HIS:CE1	1:B:523:VAL:HG23	2.46	0.51
1:E:201:MSE:CE	1:E:502:LEU:O	2.59	0.51
1:C:269:PHE:HE2	1:C:587:MSE:CE	2.21	0.51
1:E:512:ILE:HG12	1:E:538:ARG:O	2.10	0.51
1:A:526:ARG:HD2	1:A:619:VAL:HB	1.93	0.51
1:C:497:GLY:O	1:C:500:ILE:HG22	2.11	0.51
1:B:724:THR:HG22	1:B:726:THR:HG23	1.93	0.51
1:E:133:GLN:HB2	1:E:136:ASN:HD22	1.75	0.51
1:F:332:ILE:HD12	1:F:408:MSE:CE	2.36	0.51
1:E:44:ARG:HH11	1:E:44:ARG:HG3	1.75	0.51
1:F:244:GLY:O	1:F:245:PRO:C	2.49	0.51
1:C:194:TYR:CD2	1:C:466:ARG:HD3	2.46	0.51
1:D:20:LEU:HD13	1:D:38:PRO:O	2.11	0.50
1:C:262:ALA:HB3	1:C:476:PRO:CG	2.39	0.50
1:D:742:VAL:HG23	1:D:743:LYS:N	2.26	0.50
1:A:329:GLU:N	1:A:408:MSE:HE3	2.26	0.50
1:F:273:LEU:C	1:F:273:LEU:HD13	2.31	0.50
1:C:436:MSE:CE	1:C:440:TYR:HA	2.41	0.50
1:E:282:ASP:OD1	1:E:285:THR:HB	2.11	0.50
1:F:293:MSE:HG3	1:F:300:LEU:HD12	1.91	0.50
1:B:291:ASP:O	1:B:295:GLU:HG3	2.11	0.50
1:D:347:ASN:HA	1:D:444:TYR:OH	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:390:THR:HG23	1:E:429:ASP:H	1.76	0.50
1:B:748:GLN:O	1:B:749:ASP:C	2.50	0.50
1:D:347:ASN:C	1:D:347:ASN:ND2	2.64	0.50
1:E:745:ASN:C	1:E:745:ASN:HD22	2.15	0.50
1:D:18:HIS:O	1:D:38:PRO:HA	2.11	0.50
1:A:449:TRP:CH2	1:A:476:PRO:HD2	2.47	0.50
1:C:748:GLN:HB3	1:C:769:THR:HG23	1.94	0.50
1:F:282:ASP:O	1:F:286:VAL:HG23	2.11	0.50
1:A:754:GLU:HG2	1:A:759:LEU:CD2	2.42	0.50
1:B:738:LEU:HD22	1:B:738:LEU:N	2.27	0.50
1:C:664:ARG:O	1:C:667:THR:CG2	2.59	0.50
1:F:695:ASP:OD1	1:F:720:GLY:N	2.45	0.50
1:B:296:ARG:O	1:B:560:ARG:NH1	2.45	0.50
1:F:281:TYR:O	1:F:324:THR:HG23	2.11	0.50
1:C:343:CYS:HB2	1:C:412:CYS:SG	2.51	0.50
1:D:745:ASN:C	1:D:745:ASN:HD22	2.14	0.50
1:A:244:GLY:C	1:A:246:THR:N	2.65	0.50
1:E:456:VAL:HG12	1:E:460:GLU:CB	2.41	0.50
1:C:485:ALA:CB	1:C:519:ALA:HB2	2.40	0.50
1:A:73:GLN:HG3	1:C:352:GLN:NE2	2.26	0.50
1:E:344:VAL:HG21	1:E:405:LEU:HD23	1.94	0.50
1:E:456:VAL:HG12	1:E:460:GLU:HB2	1.94	0.50
1:E:61:GLN:NE2	1:E:87:LEU:CD2	2.75	0.50
1:F:405:LEU:C	1:F:410:VAL:HG22	2.33	0.50
1:A:44:ARG:HH21	1:C:278:THR:CA	2.22	0.49
1:D:265:PRO:CD	1:D:462:VAL:HG22	2.41	0.49
1:F:742:VAL:HG13	1:F:743:LYS:HG3	1.94	0.49
1:C:273:LEU:HD13	1:C:273:LEU:C	2.32	0.49
1:A:308:PHE:CD1	1:A:308:PHE:C	2.86	0.49
1:B:277:PHE:O	1:B:278:THR:CB	2.57	0.49
1:A:768:LEU:HD13	1:A:768:LEU:N	2.25	0.49
1:A:718:ARG:O	1:A:718:ARG:HG3	2.10	0.49
1:A:745:ASN:C	1:A:745:ASN:HD22	2.14	0.49
1:B:379:LYS:CA	1:B:379:LYS:HE2	2.31	0.49
1:E:416:ASP:OD1	1:E:466:ARG:HD3	2.12	0.49
1:C:416:ASP:O	1:C:416:ASP:OD2	2.30	0.49
1:E:439:HIS:HD2	3:E:1490:HOH:O	1.94	0.49
1:C:591:MSE:CE	1:C:615:MSE:HG2	2.36	0.49
1:C:646:GLY:O	1:C:647:SER:HB2	2.12	0.49
1:B:108:LEU:HD11	1:B:241:VAL:HG12	1.94	0.49
1:B:134:VAL:O	1:B:135:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:MSE:CE	1:F:502:LEU:O	2.60	0.49
1:F:201:MSE:HE2	1:F:502:LEU:O	2.12	0.49
1:D:65:VAL:HG23	1:D:108:LEU:HD13	1.94	0.49
1:E:278:THR:HG22	1:E:308:PHE:CE2	2.47	0.49
1:F:747:LEU:HD22	1:F:770:ILE:CG2	2.42	0.49
1:E:474:LYS:O	1:E:476:PRO:HD3	2.12	0.49
1:D:195:LYS:CE	1:D:478:HIS:HB3	2.43	0.49
1:A:512:ILE:HD13	1:A:528:CYS:HA	1.95	0.49
1:B:273:LEU:HD13	1:B:274:THR:N	2.28	0.49
1:E:738:LEU:HD22	1:E:738:LEU:N	2.28	0.49
1:B:665:ASP:O	1:B:667:THR:HG23	2.13	0.49
1:B:686:THR:HG23	1:B:734:TRP:HB3	1.94	0.49
1:C:725:VAL:HB	1:C:768:LEU:HD13	1.94	0.49
1:E:265:PRO:HG3	1:E:460:GLU:HA	1.95	0.49
1:D:617:ALA:HB3	1:D:660:PRO:HB2	1.95	0.49
1:D:447:LEU:HD13	1:D:447:LEU:C	2.32	0.49
1:C:568:ARG:HG2	1:C:568:ARG:HH11	1.77	0.49
1:D:262:ALA:HB3	1:D:476:PRO:CG	2.39	0.49
1:C:332:ILE:O	1:C:336:LYS:HG3	2.13	0.49
1:B:31:GLU:HG2	1:B:58:PHE:CB	2.37	0.49
1:B:689:HIS:CD2	1:B:739:ARG:NH1	2.79	0.49
1:B:100:TYR:CG	1:B:111:ARG:HD3	2.48	0.49
1:D:571:PRO:HG2	1:D:672:GLY:N	2.28	0.49
1:C:137:ASN:HB3	1:C:152:GLU:OE1	2.13	0.49
1:A:373:SER:HB3	1:E:76:LEU:CD2	2.38	0.49
1:C:244:GLY:O	1:C:246:THR:N	2.46	0.49
1:A:368:LYS:O	1:A:425:VAL:HG22	2.13	0.49
1:C:689:HIS:CE1	1:C:739:ARG:HH21	2.31	0.49
1:D:43:GLU:HB3	1:D:46:TRP:HD1	1.77	0.49
1:E:141:GLN:HA	1:E:148:ASN:HD22	1.78	0.49
1:C:474:LYS:O	1:C:476:PRO:HD3	2.12	0.48
1:C:275:THR:HG23	1:C:303:PHE:HZ	1.77	0.48
1:A:134:VAL:O	1:A:135:LYS:HB2	2.13	0.48
1:D:635:TRP:HB3	1:D:662:TYR:HB3	1.94	0.48
1:D:368:LYS:O	1:D:425:VAL:CG2	2.61	0.48
1:B:694:GLN:HB2	1:B:697:HIS:CD2	2.48	0.48
1:A:332:ILE:O	1:A:336:LYS:HG3	2.13	0.48
1:E:65:VAL:HG21	1:E:108:LEU:HD22	1.96	0.48
1:A:703:VAL:CG2	1:A:712:PHE:HB3	2.40	0.48
1:D:526:ARG:CD	1:D:619:VAL:HG22	2.43	0.48
1:E:262:ALA:HB3	1:E:476:PRO:HG2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:CG1	1:D:495:ARG:NH2	2.76	0.48
1:C:276:SER:HB2	1:C:279:THR:OG1	2.12	0.48
1:C:163:TYR:HB3	1:C:502:LEU:HD13	1.95	0.48
1:B:295:GLU:OE2	1:B:296:ARG:HG3	2.13	0.48
1:B:298:LEU:N	1:B:299:PRO:HD3	2.28	0.48
1:C:635:TRP:O	1:C:643:GLU:HA	2.14	0.48
1:E:44:ARG:HA	1:E:47:GLN:CG	2.44	0.48
1:A:41:VAL:HG22	1:A:47:GLN:CG	2.43	0.48
1:D:744:VAL:HG22	1:D:759:LEU:CD2	2.43	0.48
1:D:500:ILE:HG12	1:D:505:PHE:HB2	1.96	0.48
1:D:644:LEU:HG	1:D:650:HIS:CE1	2.48	0.48
1:B:416:ASP:OD2	1:B:466:ARG:HD3	2.13	0.48
1:F:16:LEU:HD22	1:F:140:VAL:HG22	1.94	0.48
1:E:279:THR:O	1:E:279:THR:HG22	2.13	0.48
1:E:261:PRO:HA	1:E:473:GLN:O	2.12	0.48
1:A:308:PHE:CD1	1:A:309:TRP:N	2.81	0.48
1:A:546:ARG:HG3	1:A:547:VAL:HG13	1.96	0.48
1:D:38:PRO:HG3	1:D:51:PRO:HD2	1.96	0.48
1:E:304:HIS:CD2	1:E:538:ARG:HH21	2.32	0.48
1:B:488:GLU:O	1:B:492:GLU:HG3	2.14	0.48
1:A:401:LYS:HB2	1:A:401:LYS:NZ	2.28	0.48
1:B:39:ARG:O	1:B:41:VAL:HG23	2.14	0.48
1:B:515:PHE:O	1:B:516:GLU:HB2	2.14	0.48
1:D:570:MSE:HE1	1:D:573:LEU:HD23	1.92	0.48
1:B:41:VAL:CG1	1:B:47:GLN:HG2	2.43	0.48
1:D:501:GLY:HA2	1:D:505:PHE:O	2.14	0.48
1:F:687:ALA:HA	1:F:735:THR:HG23	1.96	0.48
1:E:355:PRO:O	1:E:358:LYS:HE2	2.13	0.48
1:C:536:HIS:HA	3:C:1154:HOH:O	2.13	0.48
1:F:405:LEU:O	1:F:410:VAL:HG22	2.13	0.48
1:B:141:GLN:HA	1:B:148:ASN:HD22	1.78	0.48
1:F:425:VAL:CG1	1:F:426:GLN:H	2.26	0.48
1:C:265:PRO:HG3	1:C:459:GLU:O	2.13	0.48
1:B:651:LYS:HD3	1:B:652:GLN:N	2.29	0.48
1:E:512:ILE:HD11	1:E:531:GLY:HA3	1.95	0.47
1:F:38:PRO:HG3	1:F:51:PRO:HD2	1.95	0.47
1:D:28:GLN:HE21	1:D:28:GLN:HA	1.79	0.47
1:D:201:MSE:HE2	1:D:251:LEU:HD21	1.94	0.47
1:B:156:LEU:HD11	1:B:228:VAL:HG23	1.95	0.47
1:C:517:ASN:HA	1:C:517:ASN:HD22	1.53	0.47
1:D:591:MSE:HE1	1:D:607:GLN:C	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:ILE:HD11	1:E:338:LYS:NZ	2.28	0.47
1:A:306:ASP:C	1:A:306:ASP:OD2	2.52	0.47
1:E:733:ASN:H	1:E:733:ASN:HD22	1.59	0.47
1:A:262:ALA:HB3	1:A:476:PRO:CG	2.42	0.47
1:D:200:TYR:CE2	1:D:228:VAL:HG11	2.49	0.47
1:F:406:VAL:HA	1:F:410:VAL:HG22	1.95	0.47
1:A:321:ASP:HB3	1:A:324:THR:OG1	2.13	0.47
1:F:262:ALA:HB3	1:F:476:PRO:CG	2.43	0.47
1:D:273:LEU:HD13	1:D:274:THR:N	2.29	0.47
1:B:273:LEU:HD13	1:B:273:LEU:C	2.33	0.47
1:C:768:LEU:C	1:C:768:LEU:HD22	2.35	0.47
1:E:78:ASN:O	1:E:435:LYS:HE3	2.14	0.47
1:E:526:ARG:CZ	1:E:619:VAL:HG21	2.45	0.47
1:B:290:ILE:HD13	1:B:290:ILE:C	2.35	0.47
1:C:576:GLU:O	1:C:579:ARG:HB2	2.14	0.47
1:D:439:HIS:HD2	3:D:1125:HOH:O	1.96	0.47
1:D:712:PHE:HB2	1:D:730:GLU:O	2.13	0.47
1:A:502:LEU:CD1	1:A:592:MSE:HE2	2.29	0.47
1:A:280:ASN:HB2	1:A:308:PHE:CE2	2.50	0.47
1:A:695:ASP:HA	1:A:718:ARG:CG	2.44	0.47
1:C:186:GLY:HA3	1:C:192:GLN:HE21	1.79	0.47
1:C:200:TYR:CE2	1:C:228:VAL:HG11	2.49	0.47
1:E:447:LEU:C	1:E:447:LEU:HD13	2.35	0.47
1:D:684:GLU:CD	1:D:732:LYS:HD2	2.34	0.47
1:D:377:TRP:CE2	1:D:379:LYS:HB2	2.49	0.47
1:D:591:MSE:HE1	1:D:608:TYR:HA	1.95	0.47
1:A:279:THR:CG2	1:A:546:ARG:NH1	2.75	0.47
1:E:41:VAL:O	1:E:41:VAL:HG22	2.14	0.47
1:B:123:LEU:HD23	1:B:128:ARG:HA	1.96	0.47
1:E:101:ALA:HB3	1:E:112:VAL:CG1	2.45	0.47
1:F:275:THR:HG21	1:F:280:ASN:OD1	2.13	0.47
1:D:335:LEU:O	1:D:338:LYS:HB2	2.14	0.47
1:B:730:GLU:HG2	1:B:732:LYS:HE2	1.96	0.47
1:A:453:LYS:NZ	1:A:453:LYS:HB3	2.29	0.47
1:F:331:MSE:O	1:F:335:LEU:HG	2.14	0.47
1:A:310:MSE:CE	1:A:316:CYS:H	2.28	0.47
1:B:262:ALA:HB3	1:B:476:PRO:CG	2.43	0.47
1:C:487:TYR:OH	1:C:522:HIS:HD2	1.98	0.47
1:D:273:LEU:HD23	1:D:539:LEU:HB3	1.96	0.47
1:C:283:GLU:HA	1:C:331:MSE:HE1	1.96	0.47
1:F:377:TRP:CE2	1:F:379:LYS:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ILE:HG12	1:C:505:PHE:HB2	1.97	0.47
1:B:156:LEU:CD1	1:B:228:VAL:HG23	2.44	0.47
1:C:292:GLY:O	1:C:296:ARG:NH1	2.46	0.47
1:D:668:LEU:HD13	1:D:690:LEU:HD23	1.97	0.47
1:C:279:THR:HA	1:C:281:TYR:CZ	2.50	0.47
1:A:41:VAL:HG13	1:A:41:VAL:O	2.14	0.47
1:F:694:GLN:O	1:F:697:HIS:HB2	2.13	0.47
1:B:439:HIS:HD2	3:B:1268:HOH:O	1.98	0.47
1:E:80:PRO:HD3	1:E:431:SER:HB3	1.96	0.47
1:C:29:ASP:O	1:C:30:ASN:HB2	2.15	0.47
1:F:745:ASN:H	1:F:745:ASN:HD22	1.63	0.47
1:A:310:MSE:HE1	1:A:316:CYS:CA	2.44	0.47
1:A:279:THR:O	1:A:279:THR:CG2	2.63	0.47
1:E:243:ASP:CG	1:E:244:GLY:N	2.68	0.47
1:A:222:SER:O	1:D:191:GLU:CG	2.62	0.47
1:C:290:ILE:CD1	1:C:338:LYS:HD2	2.45	0.47
1:B:133:GLN:HB2	1:B:136:ASN:ND2	2.30	0.47
1:E:275:THR:OG1	1:E:280:ASN:ND2	2.48	0.47
1:F:364:GLY:HA2	3:F:1136:HOH:O	2.14	0.47
1:F:345:TRP:CH2	1:F:347:ASN:ND2	2.83	0.46
1:B:296:ARG:O	1:B:298:LEU:HG	2.14	0.46
1:A:500:ILE:HG12	1:A:505:PHE:HB2	1.98	0.46
1:D:419:GLU:HG3	1:D:467:SER:OG	2.15	0.46
1:E:281:TYR:O	1:E:282:ASP:HB3	2.14	0.46
1:E:744:VAL:HG21	1:E:770:ILE:CG2	2.46	0.46
1:C:225:VAL:HG11	1:F:169:PHE:O	2.15	0.46
1:F:759:LEU:C	1:F:759:LEU:HD23	2.35	0.46
1:B:651:LYS:C	1:B:651:LYS:HD3	2.36	0.46
1:C:183:ASN:HA	1:C:196:ASN:ND2	2.30	0.46
1:D:436:MSE:HE1	1:D:443:ILE:HD12	1.96	0.46
1:D:396:LYS:NZ	1:D:396:LYS:HB2	2.30	0.46
1:A:280:ASN:HB2	1:A:308:PHE:CZ	2.50	0.46
1:B:298:LEU:CD2	1:B:560:ARG:HB2	2.46	0.46
1:C:48:LEU:HD12	1:C:48:LEU:C	2.36	0.46
1:F:165:LEU:HA	1:F:197:ILE:O	2.16	0.46
1:D:382:PRO:HG3	1:F:50:THR:O	2.16	0.46
1:D:738:LEU:N	1:D:738:LEU:HD22	2.29	0.46
1:A:244:GLY:O	1:A:246:THR:N	2.49	0.46
1:D:390:THR:HG21	1:D:427:TRP:HB3	1.96	0.46
1:F:732:LYS:HE2	1:F:733:ASN:H	1.80	0.46
1:C:153:ARG:HG2	1:C:229:GLN:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:MSE:HB2	1:B:573:LEU:HD22	1.97	0.46
1:A:735:THR:HG22	1:A:762:LYS:HG2	1.98	0.46
1:B:766:ASN:O	1:B:767:ALA:HB2	2.16	0.46
1:E:292:GLY:O	1:E:296:ARG:HD3	2.16	0.46
1:F:526:ARG:CD	1:F:619:VAL:HG22	2.36	0.46
1:C:752:GLN:HB2	1:C:759:LEU:HD21	1.98	0.46
1:A:15:ASN:HB2	1:A:141:GLN:HE21	1.79	0.46
1:F:252:ASP:HA	1:F:583:ARG:O	2.14	0.46
1:A:635:TRP:HB3	1:A:662:TYR:HB3	1.98	0.46
1:C:273:LEU:HD13	1:C:274:THR:N	2.31	0.46
1:B:273:LEU:HD23	1:B:539:LEU:HB3	1.96	0.46
1:A:367:LEU:HD21	1:A:425:VAL:HG13	1.96	0.46
1:C:225:VAL:HG13	1:F:495:ARG:NH2	2.30	0.46
1:C:488:GLU:O	1:C:492:GLU:HG3	2.15	0.46
1:F:552:ASP:OD1	1:F:554:GLU:N	2.48	0.46
1:A:747:LEU:HD21	1:A:750:GLY:O	2.14	0.46
1:B:591:MSE:HE1	1:B:608:TYR:HA	1.98	0.46
1:B:248:LYS:CG	1:B:593:MSE:HE3	2.46	0.46
1:E:502:LEU:HD13	1:E:593:MSE:HE2	1.97	0.46
1:F:419:GLU:OE2	1:F:466:ARG:HD2	2.16	0.46
1:C:331:MSE:HA	1:C:334:ARG:HH11	1.79	0.46
1:B:80:PRO:HD3	1:B:431:SER:HB3	1.98	0.46
1:D:163:TYR:HB3	1:D:502:LEU:HD13	1.96	0.46
1:C:314:GLN:HB3	1:C:354:SER:HB2	1.97	0.46
1:D:384:LEU:C	1:D:384:LEU:HD23	2.36	0.46
1:B:278:THR:HG23	1:D:44:ARG:CD	2.45	0.46
1:B:714:LEU:HD21	1:B:725:VAL:HG13	1.98	0.46
1:C:195:LYS:HB3	1:C:468:ALA:HB3	1.97	0.46
1:B:664:ARG:HG3	1:B:665:ASP:N	2.30	0.46
1:B:223:GLU:O	1:E:190:THR:HA	2.16	0.46
1:E:646:GLY:O	1:E:647:SER:HB2	2.16	0.46
1:C:76:LEU:CD2	1:E:373:SER:HB3	2.33	0.46
1:A:734:TRP:CZ2	1:A:763:PRO:HG3	2.51	0.46
1:D:512:ILE:HG21	1:D:528:CYS:SG	2.55	0.46
1:C:296:ARG:HH11	1:C:296:ARG:HG3	1.79	0.46
1:D:41:VAL:HG22	1:D:47:GLN:HG2	1.98	0.46
1:C:402:LEU:HB3	1:C:451:VAL:HG11	1.98	0.46
1:B:332:ILE:HG23	1:B:342:ILE:HG13	1.97	0.46
1:F:512:ILE:N	1:F:512:ILE:HD12	2.31	0.46
1:E:635:TRP:CH2	1:E:664:ARG:HB3	2.51	0.46
1:C:296:ARG:O	1:C:298:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLU:OE2	1:A:356:VAL:HG23	2.15	0.46
1:F:736:LEU:C	1:F:736:LEU:HD13	2.36	0.46
1:A:199:PHE:HE2	1:A:201:MSE:HE2	1.81	0.45
1:D:329:GLU:CA	1:D:408:MSE:HE3	2.46	0.45
1:E:310:MSE:SE	1:E:316:CYS:H	2.48	0.45
1:E:65:VAL:CG2	1:E:108:LEU:HD22	2.46	0.45
1:D:273:LEU:C	1:D:273:LEU:HD13	2.37	0.45
1:E:137:ASN:HB3	1:E:152:GLU:OE2	2.16	0.45
1:E:183:ASN:HA	1:E:196:ASN:ND2	2.31	0.45
1:E:160:GLU:HG3	1:E:204:ARG:HG2	1.98	0.45
1:D:246:THR:HG22	1:D:249:ALA:N	2.21	0.45
1:D:310:MSE:SE	1:D:316:CYS:H	2.49	0.45
1:E:397:TRP:CZ2	1:E:401:LYS:HE2	2.52	0.45
1:C:463:LEU:O	1:C:477:VAL:HB	2.15	0.45
1:D:494:LEU:HD22	1:D:498:LEU:HG	1.98	0.45
1:C:734:TRP:CH2	1:C:763:PRO:HG2	2.51	0.45
1:F:367:LEU:HD11	1:F:425:VAL:CG1	2.44	0.45
1:B:638:LEU:HD12	1:B:639:TRP:CE3	2.50	0.45
1:E:278:THR:HG22	1:E:308:PHE:CD2	2.50	0.45
1:D:732:LYS:O	1:D:733:ASN:HB2	2.16	0.45
1:A:736:LEU:C	1:A:736:LEU:HD13	2.37	0.45
1:B:490:MSE:HE2	1:B:620:PHE:CE2	2.50	0.45
1:B:498:LEU:HD11	1:B:608:TYR:HB3	1.98	0.45
1:D:408:MSE:HE2	1:D:408:MSE:HB3	1.81	0.45
1:A:191:GLU:HB3	1:D:222:SER:O	2.17	0.45
1:B:630:LEU:O	1:B:647:SER:N	2.49	0.45
1:F:719:THR:O	1:F:719:THR:HG23	2.16	0.45
1:B:591:MSE:HE3	1:B:607:GLN:HE21	1.81	0.45
1:A:273:LEU:HB3	1:A:300:LEU:HD11	1.96	0.45
1:D:753:ALA:O	1:D:759:LEU:HD12	2.17	0.45
1:C:133:GLN:O	1:C:136:ASN:HB2	2.17	0.45
1:E:182:TRP:CE3	1:E:215:CYS:HB2	2.52	0.45
1:C:390:THR:HG21	1:C:427:TRP:HB3	1.98	0.45
1:C:748:GLN:O	1:C:749:ASP:HB2	2.17	0.45
1:A:768:LEU:C	1:A:768:LEU:HD22	2.37	0.45
1:C:449:TRP:CH2	1:C:476:PRO:HD2	2.52	0.45
1:C:283:GLU:CD	1:C:326:PRO:HD2	2.37	0.45
1:D:725:VAL:HB	1:D:768:LEU:HB2	1.97	0.45
1:D:718:ARG:HG3	1:D:723:ILE:HD13	1.99	0.45
1:F:164:GLY:O	1:F:165:LEU:HB2	2.16	0.45
1:E:265:PRO:CG	1:E:460:GLU:HA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LYS:CE	1:B:478:HIS:HB3	2.46	0.45
1:A:670:ALA:HB2	1:A:701:CYS:SG	2.57	0.45
1:C:568:ARG:NH1	1:C:568:ARG:HG2	2.32	0.45
1:A:436:MSE:HE3	1:A:440:TYR:HB2	1.97	0.45
1:F:61:GLN:HB2	1:F:64:ILE:HD12	1.99	0.45
1:B:252:ASP:HA	1:B:583:ARG:O	2.16	0.45
1:E:335:LEU:HA	1:E:335:LEU:HD13	1.86	0.45
1:A:306:ASP:OD2	1:A:308:PHE:CD2	2.69	0.45
1:B:287:ASN:CA	1:B:290:ILE:HG22	2.42	0.45
1:B:689:HIS:HD2	1:B:739:ARG:HH11	1.63	0.45
1:C:766:ASN:C	1:C:766:ASN:ND2	2.70	0.45
1:F:490:MSE:HE2	1:F:620:PHE:CD2	2.52	0.45
1:D:134:VAL:HG22	1:D:135:LYS:HG2	1.98	0.45
1:C:348:PRO:HG2	1:C:349:TYR:CE1	2.52	0.45
1:B:127:GLU:OE2	1:B:127:GLU:HA	2.16	0.45
1:E:335:LEU:O	1:E:338:LYS:HB3	2.17	0.45
1:B:524:TYR:OH	1:B:539:LEU:HD21	2.17	0.45
1:F:682:TRP:O	1:F:686:THR:HB	2.17	0.45
1:C:653:GLN:HE21	1:C:653:GLN:HB3	1.51	0.45
1:E:290:ILE:O	1:E:293:MSE:HB2	2.17	0.44
1:A:276:SER:HA	1:A:541:GLY:O	2.17	0.44
1:E:265:PRO:HD2	1:E:462:VAL:CG2	2.46	0.44
1:F:78:ASN:HB3	1:F:79:GLY:H	1.41	0.44
1:F:695:ASP:HA	1:F:718:ARG:HD3	1.99	0.44
1:B:674:ASN:HB3	1:B:680:TYR:CD1	2.52	0.44
1:A:195:LYS:HZ2	1:A:478:HIS:HB3	1.81	0.44
1:B:673:ASN:HD22	1:B:685:GLY:HA3	1.82	0.44
1:F:568:ARG:NH1	1:F:672:GLY:O	2.50	0.44
1:D:512:ILE:HD12	1:D:531:GLY:HA3	1.99	0.44
1:B:464:PHE:CE2	1:B:477:VAL:HG11	2.52	0.44
1:C:576:GLU:HG3	1:C:611:GLY:HA3	1.98	0.44
1:D:196:ASN:O	1:D:197:ILE:HD13	2.17	0.44
1:E:59:SER:HA	1:E:60:PRO:HD3	1.84	0.44
1:C:164:GLY:O	1:C:165:LEU:HB2	2.18	0.44
1:F:405:LEU:HB3	1:F:410:VAL:HG21	1.99	0.44
1:C:483:CYS:HB3	1:C:489:SER:OG	2.16	0.44
1:C:419:GLU:OE2	1:C:466:ARG:HD3	2.17	0.44
1:E:554:GLU:O	1:E:558:VAL:HG23	2.17	0.44
1:A:182:TRP:CE3	1:A:215:CYS:HB2	2.53	0.44
1:E:510:HIS:CD2	1:E:510:HIS:N	2.86	0.44
1:C:502:LEU:HD21	1:C:592:MSE:CE	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:PRO:HB2	1:B:408:MSE:HE1	1.99	0.44
1:A:18:HIS:HB2	1:A:20:LEU:HD21	1.99	0.44
1:D:25:VAL:HG21	1:D:114:LYS:HE2	1.99	0.44
1:E:67:VAL:O	1:E:238:GLU:HA	2.17	0.44
1:F:265:PRO:HG3	1:F:460:GLU:HA	1.99	0.44
1:C:591:MSE:HE3	1:C:607:GLN:HG3	1.99	0.44
1:B:755:SER:O	1:B:757:GLN:N	2.50	0.44
1:B:310:MSE:SE	1:B:316:CYS:H	2.51	0.44
1:A:194:TYR:CE2	1:A:466:ARG:HD3	2.53	0.44
1:F:230:PHE:HE1	1:F:237:LEU:HD11	1.83	0.44
1:C:436:MSE:HE3	1:C:440:TYR:N	2.32	0.44
1:B:93:THR:HG23	1:B:104:LYS:HB3	2.00	0.44
1:B:453:LYS:NZ	1:B:458:GLU:HG3	2.32	0.44
1:A:5:ASP:HB3	1:A:9:LEU:HB2	2.00	0.44
1:C:189:SER:OG	1:F:7:ASN:ND2	2.38	0.44
1:A:50:THR:O	1:C:382:PRO:HG3	2.18	0.44
1:C:276:SER:HB2	1:C:279:THR:CG2	2.48	0.44
1:F:300:LEU:HD22	1:F:340:LEU:CD2	2.43	0.44
1:F:751:SER:HB3	1:F:762:LYS:HB3	2.00	0.44
1:D:80:PRO:HD3	1:D:431:SER:HB3	1.99	0.44
1:C:278:THR:O	1:C:279:THR:HG23	2.17	0.44
1:E:635:TRP:O	1:E:643:GLU:HA	2.18	0.44
1:F:725:VAL:CG1	1:F:768:LEU:HB3	2.46	0.44
1:E:388:ASP:C	1:E:390:THR:H	2.21	0.44
1:E:575:ARG:O	1:E:578:ALA:HB3	2.18	0.44
1:D:402:LEU:HB3	1:D:451:VAL:HG11	2.00	0.44
1:D:591:MSE:CE	1:D:608:TYR:HA	2.48	0.44
1:A:279:THR:HG23	1:A:546:ARG:HH12	1.81	0.44
1:A:517:ASN:CG	1:A:518:THR:H	2.22	0.44
1:F:747:LEU:HD21	1:F:761:VAL:CG1	2.48	0.44
1:C:683:HIS:CD2	1:C:711:ILE:HD13	2.53	0.44
1:C:309:TRP:HA	1:C:325:PHE:CE1	2.53	0.44
1:E:674:ASN:HB3	1:E:680:TYR:CE1	2.53	0.44
1:A:160:GLU:HA	1:A:203:ASN:OD1	2.18	0.44
1:E:718:ARG:HD3	1:E:720:GLY:O	2.18	0.43
1:E:557:ASP:OD1	1:E:560:ARG:NH2	2.51	0.43
1:F:502:LEU:HD13	1:F:593:MSE:CE	2.48	0.43
1:E:539:LEU:HD23	1:E:540:HIS:N	2.33	0.43
1:B:648:ARG:HH11	1:B:648:ARG:HG3	1.83	0.43
1:F:747:LEU:HD21	1:F:761:VAL:HG13	2.00	0.43
1:F:200:TYR:CE2	1:F:228:VAL:HG11	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ASP:HA	1:A:599:PRO:HD3	1.84	0.43
1:E:748:GLN:HB3	1:E:748:GLN:HE21	1.60	0.43
1:C:495:ARG:HH21	1:F:225:VAL:HG11	1.81	0.43
1:D:300:LEU:HD12	1:D:340:LEU:HD21	1.97	0.43
1:D:734:TRP:CH2	1:D:763:PRO:HG3	2.53	0.43
1:B:137:ASN:HB3	1:B:152:GLU:OE1	2.18	0.43
1:F:598:ASP:HA	1:F:599:PRO:HD3	1.89	0.43
1:E:154:LEU:HA	1:E:154:LEU:HD12	1.84	0.43
1:E:475:PHE:N	1:E:476:PRO:HD3	2.32	0.43
1:E:16:LEU:CD2	1:E:140:VAL:HG22	2.45	0.43
1:B:531:GLY:O	1:B:537:SER:HB3	2.18	0.43
1:C:617:ALA:O	1:C:660:PRO:HD2	2.18	0.43
1:F:134:VAL:O	1:F:135:LYS:HB2	2.18	0.43
1:E:191:GLU:OE2	1:E:191:GLU:N	2.44	0.43
1:F:265:PRO:HD2	1:F:462:VAL:CG2	2.38	0.43
1:F:449:TRP:CH2	1:F:476:PRO:HD2	2.54	0.43
1:E:526:ARG:HD2	1:E:619:VAL:CG2	2.40	0.43
1:E:723:ILE:HB	1:E:770:ILE:HB	2.01	0.43
1:C:744:VAL:HG11	1:C:770:ILE:CD1	2.48	0.43
1:C:723:ILE:HB	1:C:770:ILE:HG23	1.99	0.43
1:F:568:ARG:HH11	1:F:568:ARG:HG2	1.84	0.43
1:A:137:ASN:HB3	1:A:152:GLU:OE1	2.18	0.43
1:D:488:GLU:O	1:D:492:GLU:HG3	2.18	0.43
1:D:668:LEU:O	1:D:701:CYS:HB2	2.18	0.43
1:B:354:SER:HA	1:B:355:PRO:HD3	1.92	0.43
1:F:277:PHE:CD2	1:F:278:THR:HG23	2.54	0.43
1:C:290:ILE:O	1:C:293:MSE:HB2	2.18	0.43
1:A:695:ASP:HA	1:A:718:ARG:HG3	2.00	0.43
1:D:744:VAL:HG22	1:D:759:LEU:HD21	2.00	0.43
1:A:754:GLU:HG2	1:A:759:LEU:HD21	2.01	0.43
1:F:743:LYS:HA	1:F:759:LEU:HD12	1.99	0.43
1:C:768:LEU:H	1:C:768:LEU:HD13	1.83	0.43
1:C:219:GLU:HB2	1:C:229:GLN:HB3	2.00	0.43
1:D:104:LYS:HE2	1:D:106:GLY:O	2.19	0.43
1:A:348:PRO:HD3	1:A:444:TYR:CZ	2.53	0.43
1:B:18:HIS:O	1:B:38:PRO:HA	2.18	0.43
1:D:735:THR:OG1	1:D:760:VAL:HG13	2.19	0.43
1:A:745:ASN:ND2	1:A:745:ASN:C	2.72	0.43
1:B:510:HIS:CD2	1:B:510:HIS:N	2.87	0.43
1:A:673:ASN:N	1:A:673:ASN:HD22	2.14	0.43
1:A:498:LEU:O	1:A:502:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:SER:O	1:B:756:GLU:C	2.57	0.43
1:A:734:TRP:CH2	1:A:763:PRO:HG3	2.53	0.43
1:E:244:GLY:CA	1:E:253:ARG:HH12	2.31	0.43
1:E:745:ASN:O	1:E:745:ASN:ND2	2.52	0.43
1:A:136:ASN:HB3	1:A:153:ARG:HB2	2.00	0.43
1:E:479:TRP:CZ3	1:E:481:GLY:HA2	2.53	0.43
1:E:500:ILE:HG12	1:E:505:PHE:HB2	1.99	0.43
1:C:730:GLU:HA	1:C:730:GLU:OE2	2.19	0.43
1:A:447:LEU:C	1:A:447:LEU:HD13	2.39	0.43
1:D:401:LYS:HA	1:D:401:LYS:HD3	1.81	0.43
1:A:251:LEU:HD11	1:A:593:MSE:HE2	2.00	0.43
1:C:282:ASP:H	1:C:285:THR:HG21	1.81	0.43
1:B:557:ASP:OD2	1:B:560:ARG:NH2	2.52	0.43
1:B:246:THR:OG1	1:B:247:PRO:HD2	2.19	0.43
1:B:313:PHE:HZ	1:D:41:VAL:HG21	1.84	0.43
1:E:336:LYS:O	1:E:337:ALA:C	2.54	0.43
1:F:475:PHE:N	1:F:476:PRO:HD3	2.33	0.43
1:D:283:GLU:HA	1:D:331:MSE:HE3	2.01	0.43
1:D:246:THR:HG22	1:D:249:ALA:CB	2.49	0.43
1:E:367:LEU:HD13	1:E:425:VAL:HG21	2.01	0.43
1:B:29:ASP:CG	1:B:30:ASN:N	2.71	0.43
1:C:286:VAL:HG11	1:C:331:MSE:HE1	2.01	0.43
1:C:768:LEU:H	1:C:768:LEU:CD1	2.31	0.43
1:A:320:TRP:O	1:A:322:PRO:HD3	2.19	0.43
1:A:165:LEU:HA	1:A:197:ILE:O	2.19	0.43
1:E:498:LEU:O	1:E:502:LEU:HD22	2.19	0.42
1:A:377:TRP:HH2	1:A:420:ARG:HD3	1.82	0.42
1:F:635:TRP:HB3	1:F:662:TYR:HB3	2.00	0.42
1:A:28:GLN:O	1:A:29:ASP:HB2	2.19	0.42
1:A:306:ASP:O	1:A:309:TRP:HD1	2.03	0.42
1:E:720:GLY:C	1:E:721:ASN:HD22	2.22	0.42
1:D:152:GLU:HB3	1:D:230:PHE:CE1	2.54	0.42
1:F:379:LYS:O	1:F:380:TRP:HB3	2.19	0.42
1:D:745:ASN:H	1:D:745:ASN:ND2	2.17	0.42
1:C:641:ASN:OD1	1:C:739:ARG:HD2	2.18	0.42
1:A:348:PRO:HG2	1:A:349:TYR:CE2	2.54	0.42
1:A:200:TYR:CE2	1:A:228:VAL:HG11	2.53	0.42
1:B:384:LEU:HD23	1:B:384:LEU:C	2.40	0.42
1:D:264:PRO:HG3	1:D:476:PRO:HB3	2.01	0.42
1:F:290:ILE:HD13	1:F:340:LEU:CD1	2.50	0.42
1:E:244:GLY:O	1:E:245:PRO:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:THR:HG22	1:C:428:PHE:HB3	2.01	0.42
1:D:356:VAL:HG23	1:D:359:GLU:OE2	2.19	0.42
1:F:312:ALA:O	1:F:313:PHE:HB2	2.19	0.42
1:C:275:THR:HG23	1:C:303:PHE:CZ	2.53	0.42
1:C:627:GLN:NE2	1:F:599:PRO:HG3	2.34	0.42
1:A:342:ILE:CG1	1:A:410:VAL:HA	2.49	0.42
1:B:172:LEU:HD22	3:B:1047:HOH:O	2.19	0.42
1:E:219:GLU:HB2	1:E:229:GLN:HB3	2.01	0.42
1:A:2:LYS:HA	1:A:2:LYS:HD3	1.74	0.42
1:C:87:LEU:N	1:C:87:LEU:HD22	2.35	0.42
1:C:16:LEU:CD2	1:C:140:VAL:HG22	2.47	0.42
1:D:378:ASP:OD2	1:F:71:HIS:HE1	2.02	0.42
1:B:41:VAL:HG11	1:F:313:PHE:HZ	1.84	0.42
1:A:139:TYR:CD1	1:A:150:MSE:HE1	2.55	0.42
1:B:750:GLY:HA2	1:B:764:GLN:H	1.83	0.42
1:B:2:LYS:HA	1:B:223:GLU:OE2	2.18	0.42
1:C:617:ALA:HB3	1:C:660:PRO:HB2	2.01	0.42
1:D:479:TRP:CZ3	1:D:481:GLY:HA2	2.54	0.42
1:B:641:ASN:ND2	1:B:757:GLN:CG	2.71	0.42
1:F:627:GLN:HA	1:F:650:HIS:O	2.20	0.42
1:C:591:MSE:HE2	1:C:608:TYR:HA	2.00	0.42
1:F:237:LEU:C	1:F:237:LEU:HD13	2.40	0.42
1:C:225:VAL:CG1	1:F:495:ARG:HH21	2.33	0.42
1:C:490:MSE:HE2	1:C:620:PHE:CE2	2.55	0.42
1:D:320:TRP:O	1:D:322:PRO:HD3	2.20	0.42
1:B:76:LEU:HG	1:F:373:SER:HB3	2.02	0.42
1:A:310:MSE:HB3	1:A:310:MSE:HE2	1.89	0.42
1:A:310:MSE:CE	1:A:318:PHE:H	2.32	0.42
1:B:570:MSE:HG3	1:B:678:PRO:HA	2.02	0.42
1:C:348:PRO:HD3	1:C:444:TYR:CZ	2.55	0.42
1:E:306:ASP:HA	2:E:805:MES:O2S	2.19	0.42
1:B:273:LEU:HD11	1:B:289:PHE:CE1	2.55	0.42
1:A:299:PRO:HB3	1:A:676:GLN:O	2.20	0.42
1:A:588:MSE:HG3	1:A:608:TYR:CD2	2.54	0.42
1:E:277:PHE:C	1:E:278:THR:HG23	2.40	0.42
1:D:685:GLY:HA2	1:D:733:ASN:O	2.20	0.42
1:B:64:ILE:CD1	1:B:242:ILE:HD12	2.50	0.42
1:E:582:ALA:O	1:E:583:ARG:HD2	2.20	0.42
1:A:310:MSE:HE1	1:A:318:PHE:H	1.85	0.42
1:D:715:LYS:HG2	1:D:716:ALA:N	2.34	0.42
1:C:123:LEU:HD13	1:C:128:ARG:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:GLU:HB2	1:B:229:GLN:HB3	2.02	0.42
1:B:225:VAL:CG1	1:E:492:GLU:HG2	2.49	0.42
1:A:342:ILE:HG13	1:A:410:VAL:HA	2.01	0.42
1:D:1:MSE:HE1	1:D:149:TYR:CZ	2.55	0.42
1:B:521:ALA:O	1:B:525:LYS:HG3	2.20	0.42
1:C:364:GLY:HA2	3:C:1069:HOH:O	2.19	0.42
1:E:41:VAL:CG2	1:E:47:GLN:HA	2.50	0.42
1:B:539:LEU:HB3	1:B:540:HIS:H	1.73	0.42
1:C:225:VAL:HG13	1:F:495:ARG:HH21	1.84	0.42
1:E:208:VAL:HA	1:E:240:PHE:O	2.20	0.42
1:C:43:GLU:O	1:C:45:THR:O	2.38	0.42
1:A:282:ASP:OD2	1:A:285:THR:HG23	2.20	0.42
1:B:591:MSE:HE1	1:B:607:GLN:C	2.40	0.41
1:E:296:ARG:HB3	1:E:298:LEU:HD23	2.01	0.41
1:D:519:ALA:HB3	1:D:520:PRO:CD	2.41	0.41
1:D:589:ARG:HG2	1:D:593:MSE:SE	2.70	0.41
1:E:273:LEU:HD21	1:E:289:PHE:HE1	1.82	0.41
1:A:718:ARG:HD2	1:A:720:GLY:O	2.19	0.41
1:C:380:TRP:HH2	2:C:803:MES:H21	1.83	0.41
1:D:71:HIS:CD2	1:D:235:GLU:OE1	2.72	0.41
1:B:416:ASP:O	1:B:416:ASP:OD2	2.38	0.41
1:E:377:TRP:CE2	1:E:379:LYS:HB2	2.55	0.41
1:E:295:GLU:C	1:E:297:ASN:N	2.74	0.41
1:A:300:LEU:HA	1:A:300:LEU:HD22	1.90	0.41
1:F:566:LYS:HA	1:F:569:MSE:CE	2.45	0.41
1:A:308:PHE:C	1:A:308:PHE:HD1	2.23	0.41
1:B:331:MSE:HA	1:B:334:ARG:NH1	2.35	0.41
1:E:136:ASN:HB3	1:E:153:ARG:HB2	2.01	0.41
1:A:742:VAL:O	1:A:759:LEU:HD23	2.21	0.41
1:C:296:ARG:NH1	1:C:296:ARG:HG3	2.35	0.41
1:D:641:ASN:HD21	1:D:757:GLN:HG2	1.85	0.41
1:A:323:LEU:HD22	1:A:323:LEU:N	2.35	0.41
1:C:55:LEU:HG	1:C:69:ILE:HG12	2.02	0.41
1:D:570:MSE:HG3	1:D:678:PRO:HA	2.02	0.41
1:F:137:ASN:HB3	1:F:152:GLU:CD	2.41	0.41
1:B:539:LEU:O	1:B:540:HIS:CB	2.68	0.41
1:A:20:LEU:O	1:A:118:TRP:HB2	2.21	0.41
1:F:220:VAL:HG13	1:F:228:VAL:HG22	2.00	0.41
1:C:384:LEU:HD23	1:C:384:LEU:C	2.41	0.41
1:C:535:SER:CA	1:C:587:MSE:HE3	2.49	0.41
1:C:524:TYR:OH	1:C:539:LEU:HD11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:LEU:O	1:B:464:PHE:HD2	2.03	0.41
1:E:388:ASP:OD1	1:E:390:THR:HB	2.20	0.41
1:D:352:GLN:NE2	1:F:73:GLN:HG3	2.35	0.41
1:E:552:ASP:N	1:E:555:SER:HG	2.18	0.41
1:D:76:LEU:HD12	1:D:76:LEU:HA	1.82	0.41
1:F:669:LEU:HA	1:F:669:LEU:HD23	1.92	0.41
1:F:425:VAL:HG13	1:F:426:GLN:H	1.86	0.41
1:C:665:ASP:O	1:C:667:THR:HG22	2.21	0.41
1:A:689:HIS:CD2	1:A:739:ARG:HD3	2.52	0.41
1:C:272:TRP:HB2	1:C:538:ARG:HA	2.01	0.41
1:A:752:GLN:HB2	1:A:759:LEU:CD1	2.51	0.41
1:E:358:LYS:O	1:E:362:GLU:HG3	2.21	0.41
1:C:20:LEU:O	1:C:118:TRP:HB2	2.21	0.41
1:F:345:TRP:HH2	1:F:347:ASN:ND2	2.18	0.41
1:A:306:ASP:OD2	1:A:307:CYS:N	2.54	0.41
1:D:749:ASP:O	1:D:763:PRO:HA	2.21	0.41
1:B:378:ASP:OD1	1:D:71:HIS:HE1	2.04	0.41
1:A:342:ILE:HD11	1:A:410:VAL:HG12	2.03	0.41
1:C:80:PRO:HD3	1:C:431:SER:HB3	2.02	0.41
1:C:610:LEU:HA	1:C:610:LEU:HD23	1.94	0.41
1:A:318:PHE:HB2	1:A:401:LYS:HG2	2.02	0.41
1:E:290:ILE:HD11	1:E:338:LYS:HZ2	1.85	0.41
1:F:262:ALA:O	1:F:264:PRO:HD3	2.21	0.41
1:C:281:TYR:N	1:C:285:THR:HG21	2.35	0.41
1:B:475:PHE:N	1:B:476:PRO:HD3	2.34	0.41
1:D:309:TRP:CE2	1:D:310:MSE:HE2	2.55	0.41
1:C:121:ASP:OD1	1:C:128:ARG:HD2	2.20	0.41
1:F:232:VAL:HG12	1:F:237:LEU:HD23	2.03	0.41
1:A:265:PRO:HG3	1:A:459:GLU:O	2.20	0.41
1:F:246:THR:HG23	1:F:249:ALA:CB	2.50	0.41
1:D:82:TYR:CE2	1:D:470:VAL:HB	2.55	0.41
1:C:173:VAL:HB	3:C:1086:HOH:O	2.20	0.41
1:F:182:TRP:CE3	1:F:215:CYS:HB2	2.55	0.41
1:B:649:TRP:CD1	1:E:600:ALA:HB2	2.55	0.41
1:F:358:LYS:HE2	1:F:358:LYS:HB3	1.91	0.41
1:B:591:MSE:CE	1:B:608:TYR:HA	2.51	0.41
1:E:286:VAL:O	1:E:290:ILE:HG23	2.21	0.41
1:F:569:MSE:HB2	1:F:573:LEU:HD22	2.02	0.41
1:A:518:THR:CG2	1:A:519:ALA:H	2.28	0.41
1:C:262:ALA:HB3	1:C:476:PRO:CD	2.51	0.41
1:F:723:ILE:HB	1:F:770:ILE:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:THR:HA	1:D:541:GLY:HA3	2.02	0.41
1:C:506:GLY:HA2	1:C:586:PRO:HA	2.02	0.41
1:C:327:ASP:OD2	1:C:330:GLY:HA3	2.20	0.41
1:F:664:ARG:HG2	1:F:665:ASP:N	2.36	0.41
1:A:380:TRP:CH2	2:A:801:MES:H21	2.55	0.41
1:A:533:LEU:HA	1:A:533:LEU:HD12	1.85	0.41
1:F:354:SER:HA	1:F:355:PRO:HD3	1.90	0.41
1:D:354:SER:HA	1:D:355:PRO:HD3	1.86	0.41
1:B:273:LEU:HD23	1:B:539:LEU:HD13	2.03	0.41
1:B:41:VAL:HG12	1:B:47:GLN:CG	2.50	0.41
1:B:764:GLN:O	1:B:764:GLN:HG3	2.19	0.41
1:A:296:ARG:HD2	1:A:549:TRP:CZ3	2.56	0.41
1:B:161:THR:O	1:B:202:THR:HA	2.20	0.41
1:F:17:ILE:HG13	1:F:53:PHE:HZ	1.85	0.41
1:F:510:HIS:CD2	1:F:510:HIS:N	2.89	0.41
1:B:31:GLU:OE1	1:B:56:ARG:HD3	2.21	0.41
1:D:283:GLU:HA	1:D:331:MSE:HE1	2.02	0.41
1:A:519:ALA:O	1:A:551:TYR:HE2	2.04	0.41
1:D:273:LEU:HD22	1:D:274:THR:H	1.86	0.41
1:B:243:ASP:CG	1:B:244:GLY:H	2.25	0.41
1:F:745:ASN:HD22	1:F:745:ASN:C	2.24	0.41
1:F:745:ASN:HD22	1:F:745:ASN:N	2.19	0.41
1:F:341:LYS:O	1:F:342:ILE:HD12	2.21	0.41
1:C:267:TRP:CE3	1:C:341:LYS:HG3	2.56	0.41
1:E:609:MSE:HE2	1:E:609:MSE:CA	2.49	0.40
1:B:377:TRP:NE1	1:B:379:LYS:HB2	2.36	0.40
1:C:408:MSE:HE2	1:C:408:MSE:HB3	1.96	0.40
1:C:512:ILE:HD12	1:C:539:LEU:HD22	2.02	0.40
1:B:744:VAL:HG11	1:B:770:ILE:CG2	2.51	0.40
1:B:772:LEU:H	1:B:772:LEU:CD2	2.31	0.40
1:E:749:ASP:C	1:E:764:GLN:HG2	2.42	0.40
1:C:199:PHE:CE2	1:C:201:MSE:HG3	2.56	0.40
1:F:78:ASN:HA	1:F:78:ASN:HD22	1.70	0.40
1:B:569:MSE:CB	1:B:573:LEU:HD22	2.51	0.40
1:C:306:ASP:O	1:C:309:TRP:HD1	2.04	0.40
1:C:381:GLN:CA	1:C:381:GLN:HE21	2.34	0.40
1:A:306:ASP:CG	1:A:308:PHE:CD2	2.95	0.40
1:A:79:GLY:HA3	1:A:432:ASP:HB3	2.03	0.40
1:D:156:LEU:HD13	1:D:228:VAL:HG23	2.03	0.40
1:A:20:LEU:HD22	1:A:134:VAL:CG2	2.50	0.40
1:E:221:GLY:HA2	1:E:224:LYS:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:408:MSE:HB3	1:F:408:MSE:HE2	1.92	0.40
1:A:314:GLN:HB2	1:A:354:SER:CB	2.44	0.40
1:E:309:TRP:CE2	1:E:310:MSE:HE2	2.57	0.40
1:A:495:ARG:HH21	1:D:225:VAL:CG1	2.33	0.40
1:B:183:ASN:HA	1:B:196:ASN:ND2	2.36	0.40
1:E:271:LEU:HD13	1:E:271:LEU:O	2.22	0.40
1:A:579:ARG:HH21	1:A:579:ARG:HG2	1.87	0.40
1:F:264:PRO:HA	1:F:265:PRO:HD3	1.83	0.40
1:A:275:THR:O	1:A:276:SER:C	2.59	0.40
1:F:195:LYS:CE	1:F:478:HIS:HB3	2.45	0.40
1:A:475:PHE:N	1:A:476:PRO:HD3	2.36	0.40
1:E:347:ASN:HB2	1:E:348:PRO:HD2	2.03	0.40
1:E:326:PRO:O	1:E:328:PRO:HD3	2.21	0.40
1:D:754:GLU:OE2	1:D:759:LEU:HD13	2.21	0.40
1:C:748:GLN:HB3	1:C:769:THR:HG22	2.03	0.40
1:A:497:GLY:C	1:A:588:MSE:HE2	2.41	0.40
1:C:39:ARG:NH2	1:C:50:THR:HB	2.37	0.40
1:B:312:ALA:O	1:B:313:PHE:HB2	2.22	0.40
1:A:19:PRO:HD2	1:A:137:ASN:OD1	2.22	0.40
1:E:669:LEU:HD13	1:E:670:ALA:N	2.37	0.40
1:A:381:GLN:HB2	1:A:384:LEU:HD12	2.03	0.40
1:A:674:ASN:HB3	1:A:680:TYR:CZ	2.57	0.40
1:E:293:MSE:HE2	1:E:296:ARG:NH2	2.37	0.40
1:D:749:ASP:HB3	1:D:764:GLN:HG3	2.03	0.40
1:A:43:GLU:CD	1:A:46:TRP:HD1	2.25	0.40
1:A:43:GLU:CG	1:A:46:TRP:CD1	3.05	0.40
1:B:153:ARG:HG2	1:B:229:GLN:HB2	2.04	0.40
1:C:598:ASP:HA	1:C:599:PRO:HD3	1.86	0.40
1:A:17:ILE:HG13	1:A:53:PHE:HZ	1.86	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	770/772 (100%)	722 (94%)	39 (5%)	9 (1%)	16	23
1	B	756/772 (98%)	702 (93%)	40 (5%)	14 (2%)	10	12
1	C	750/772 (97%)	695 (93%)	46 (6%)	9 (1%)	16	23
1	D	751/772 (97%)	700 (93%)	39 (5%)	12 (2%)	12	16
1	E	749/772 (97%)	696 (93%)	45 (6%)	8 (1%)	17	25
1	F	751/772 (97%)	703 (94%)	38 (5%)	10 (1%)	15	21
All	All	4527/4632 (98%)	4218 (93%)	247 (6%)	62 (1%)	14	19

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ASP
1	B	539	LEU
1	B	749	ASP
1	B	767	ALA
1	C	29	ASP
1	D	29	ASP
1	D	277	PHE
1	D	748	GLN
1	F	482	ASP
1	A	316	CYS
1	A	517	ASN
1	A	766	ASN
1	B	516	GLU
1	C	280	ASN
1	C	476	PRO
1	D	476	PRO
1	D	541	GLY
1	E	29	ASP
1	E	79	GLY
1	E	476	PRO
1	E	729	GLY
1	E	768	LEU
1	F	339	GLY
1	B	476	PRO
1	B	518	THR
1	B	756	GLU
1	F	79	GLY
1	B	278	THR
1	B	316	CYS
1	B	692	ASN

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Mol	Chain	Res	Type
1	B	753	ALA
1	C	316	CYS
1	D	78	ASN
1	D	731	ALA
1	D	751	SER
1	E	338	LYS
1	F	476	PRO
1	F	749	ASP
1	A	477	VAL
1	A	692	ASN
1	B	477	VAL
1	C	692	ASN
1	D	477	VAL
1	E	477	VAL
1	E	749	ASP
1	F	316	CYS
1	F	477	VAL
1	C	244	GLY
1	C	477	VAL
1	D	79	GLY
1	F	483	CYS
1	A	79	GLY
1	B	245	PRO
1	F	245	PRO
1	A	328	PRO
1	A	476	PRO
1	F	244	GLY
1	C	245	PRO
1	D	681	VAL
1	D	765	GLY
1	A	244	GLY
1	C	225	VAL

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	659/640 (103%)	613 (93%)	46 (7%)	19	29
1	B	649/640 (101%)	608 (94%)	41 (6%)	22	35
1	C	647/640 (101%)	602 (93%)	45 (7%)	19	29
1	D	647/640 (101%)	602 (93%)	45 (7%)	19	29
1	E	646/640 (101%)	605 (94%)	41 (6%)	22	35
1	F	646/640 (101%)	610 (94%)	36 (6%)	26	41
All	All	3894/3840 (101%)	3640 (94%)	254 (6%)	21	33

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	43	GLU
1	A	46	TRP
1	A	48	LEU
1	A	76	LEU
1	A	123	LEU
1	A	125	ASN
1	A	156	LEU
1	A	165	LEU
1	A	237	LEU
1	A	246	THR
1	A	263	LEU
1	A	300	LEU
1	A	308	PHE
1	A	316	CYS
1	A	347	ASN
1	A	360	LEU
1	A	367	LEU
1	A	377	TRP
1	A	393	ASP
1	A	401	LYS
1	A	402	LEU
1	A	425	VAL
1	A	452	LEU
1	A	462	VAL
1	A	464	PHE
1	A	510	HIS
1	A	517	ASN
1	A	527	TRP
1	A	533	LEU

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Mol	Chain	Res	Type
1	A	537	SER
1	A	538	ARG
1	A	573	LEU
1	A	592	MSE
1	A	604	LEU
1	A	653	GLN
1	A	668	LEU
1	A	673	ASN
1	A	686	THR
1	A	704	PRO
1	A	718	ARG
1	A	745	ASN
1	A	747	LEU
1	A	759	LEU
1	A	768	LEU
1	A	769	THR
1	B	9	LEU
1	B	48	LEU
1	B	60	PRO
1	B	108	LEU
1	B	116	GLU
1	B	120	LEU
1	B	156	LEU
1	B	165	LEU
1	B	172	LEU
1	B	263	LEU
1	B	290	ILE
1	B	295	GLU
1	B	300	LEU
1	B	316	CYS
1	B	367	LEU
1	B	377	TRP
1	B	452	LEU
1	B	473	GLN
1	B	476	PRO
1	B	494	LEU
1	B	498	LEU
1	B	510	HIS
1	B	516	GLU
1	B	539	LEU
1	B	573	LEU
1	B	589	ARG

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Mol	Chain	Res	Type
1	B	592	MSE
1	B	597	ASP
1	B	604	LEU
1	B	619	VAL
1	B	677	ARG
1	B	681	VAL
1	B	682	TRP
1	B	683	HIS
1	B	686	THR
1	B	704	PRO
1	B	711	ILE
1	B	714	LEU
1	B	719	THR
1	B	736	LEU
1	B	756	GLU
1	C	2	LYS
1	C	41	VAL
1	C	46	TRP
1	C	47	GLN
1	C	49	ASP
1	C	88	GLN
1	C	120	LEU
1	C	123	LEU
1	C	156	LEU
1	C	165	LEU
1	C	251	LEU
1	C	275	THR
1	C	286	VAL
1	C	298	LEU
1	C	316	CYS
1	C	340	LEU
1	C	377	TRP
1	C	381	GLN
1	C	390	THR
1	C	402	LEU
1	C	452	LEU
1	C	462	VAL
1	C	464	PHE
1	C	466	ARG
1	C	476	PRO
1	C	510	HIS
1	C	517	ASN

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Mol	Chain	Res	Type
1	C	537	SER
1	C	539	LEU
1	C	540	HIS
1	C	589	ARG
1	C	610	LEU
1	C	619	VAL
1	C	653	GLN
1	C	667	THR
1	C	673	ASN
1	C	677	ARG
1	C	686	THR
1	C	693	LEU
1	C	710	VAL
1	C	745	ASN
1	C	749	ASP
1	C	766	ASN
1	C	768	LEU
1	C	770	ILE
1	D	43	GLU
1	D	76	LEU
1	D	108	LEU
1	D	120	LEU
1	D	123	LEU
1	D	156	LEU
1	D	165	LEU
1	D	191	GLU
1	D	246	THR
1	D	278	THR
1	D	300	LEU
1	D	316	CYS
1	D	342	ILE
1	D	347	ASN
1	D	377	TRP
1	D	390	THR
1	D	402	LEU
1	D	458	GLU
1	D	459	GLU
1	D	462	VAL
1	D	463	LEU
1	D	464	PHE
1	D	467	SER
1	D	476	PRO

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Mol	Chain	Res	Type
1	D	494	LEU
1	D	537	SER
1	D	539	LEU
1	D	540	HIS
1	D	552	ASP
1	D	553	ASP
1	D	573	LEU
1	D	592	MSE
1	D	604	LEU
1	D	630	LEU
1	D	638	LEU
1	D	644	LEU
1	D	684	GLU
1	D	686	THR
1	D	704	PRO
1	D	732	LYS
1	D	735	THR
1	D	743	LYS
1	D	745	ASN
1	D	747	LEU
1	D	764	GLN
1	E	84	LEU
1	E	108	LEU
1	E	120	LEU
1	E	154	LEU
1	E	156	LEU
1	E	165	LEU
1	E	172	LEU
1	E	263	LEU
1	E	300	LEU
1	E	316	CYS
1	E	342	ILE
1	E	347	ASN
1	E	360	LEU
1	E	367	LEU
1	E	377	TRP
1	E	390	THR
1	E	452	LEU
1	E	462	VAL
1	E	463	LEU
1	E	464	PHE
1	E	476	PRO

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Mol	Chain	Res	Type
1	E	494	LEU
1	E	502	LEU
1	E	537	SER
1	E	573	LEU
1	E	583	ARG
1	E	592	MSE
1	E	619	VAL
1	E	634	ARG
1	E	638	LEU
1	E	651	LYS
1	E	686	THR
1	E	718	ARG
1	E	730	GLU
1	E	733	ASN
1	E	736	LEU
1	E	745	ASN
1	E	748	GLN
1	E	749	ASP
1	E	754	GLU
1	E	759	LEU
1	F	1	MSE
1	F	30	ASN
1	F	49	ASP
1	F	91	LYS
1	F	156	LEU
1	F	165	LEU
1	F	248	LYS
1	F	251	LEU
1	F	271	LEU
1	F	316	CYS
1	F	333	ARG
1	F	350	ILE
1	F	360	LEU
1	F	377	TRP
1	F	405	LEU
1	F	463	LEU
1	F	464	PHE
1	F	498	LEU
1	F	510	HIS
1	F	527	TRP
1	F	573	LEU
1	F	575	ARG

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Mol	Chain	Res	Type
1	F	592	MSE
1	F	604	LEU
1	F	610	LEU
1	F	613	ASN
1	F	619	VAL
1	F	676	GLN
1	F	686	THR
1	F	693	LEU
1	F	726	THR
1	F	732	LYS
1	F	735	THR
1	F	743	LYS
1	F	745	ASN
1	F	747	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	18	HIS
1	A	27	GLN
1	A	28	GLN
1	A	88	GLN
1	A	107	ASN
1	A	125	ASN
1	A	141	GLN
1	A	146	GLN
1	A	192	GLN
1	A	280	ASN
1	A	287	ASN
1	A	439	HIS
1	A	450	ASN
1	A	517	ASN
1	A	540	HIS
1	A	613	ASN
1	A	653	GLN
1	A	673	ASN
1	A	689	HIS
1	A	721	ASN
1	A	733	ASN
1	A	745	ASN
1	B	15	ASN

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Mol	Chain	Res	Type
1	B	27	GLN
1	B	28	GLN
1	B	73	GLN
1	B	78	ASN
1	B	107	ASN
1	B	125	ASN
1	B	141	GLN
1	B	148	ASN
1	B	192	GLN
1	B	361	GLN
1	B	439	HIS
1	B	450	ASN
1	B	564	GLN
1	B	613	ASN
1	B	689	HIS
1	B	697	HIS
1	B	748	GLN
1	C	15	ASN
1	C	28	GLN
1	C	73	GLN
1	C	77	ASN
1	C	107	ASN
1	C	125	ASN
1	C	141	GLN
1	C	146	GLN
1	C	192	GLN
1	C	445	ASN
1	C	450	ASN
1	C	517	ASN
1	C	522	HIS
1	C	627	GLN
1	C	653	GLN
1	C	673	ASN
1	C	697	HIS
1	C	733	ASN
1	C	745	ASN
1	C	766	ASN
1	D	28	GLN
1	D	71	HIS
1	D	88	GLN
1	D	192	GLN
1	D	347	ASN

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Mol	Chain	Res	Type
1	D	434	GLN
1	D	439	HIS
1	D	445	ASN
1	D	564	GLN
1	D	627	GLN
1	D	697	HIS
1	D	733	ASN
1	D	745	ASN
1	D	752	GLN
1	D	757	GLN
1	E	11	GLN
1	E	27	GLN
1	E	28	GLN
1	E	73	GLN
1	E	78	ASN
1	E	88	GLN
1	E	146	GLN
1	E	148	ASN
1	E	280	ASN
1	E	347	ASN
1	E	361	GLN
1	E	613	ASN
1	E	721	ASN
1	E	733	ASN
1	E	745	ASN
1	E	748	GLN
1	F	7	ASN
1	F	18	HIS
1	F	71	HIS
1	F	77	ASN
1	F	78	ASN
1	F	107	ASN
1	F	125	ASN
1	F	564	GLN
1	F	627	GLN
1	F	676	GLN
1	F	697	HIS
1	F	745	ASN
1	F	748	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	MES	A	801	-	11,12,12	0.58	0	14,16,16	0.98	2 (14%)
2	MES	B	802	-	11,12,12	0.51	0	14,16,16	0.84	1 (7%)
2	MES	C	803	-	11,12,12	0.44	0	14,16,16	0.80	0
2	MES	D	804	-	11,12,12	0.50	0	14,16,16	0.88	1 (7%)
2	MES	E	805	-	11,12,12	0.50	0	14,16,16	0.77	0
2	MES	F	806	-	11,12,12	0.43	0	14,16,16	1.37	2 (14%)

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	MES	A	801	-	-	0/6/14/14	0/1/1/1
2	MES	B	802	-	-	0/6/14/14	0/1/1/1
2	MES	C	803	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	D	804	-	-	0/6/14/14	0/1/1/1
2	MES	E	805	-	-	0/6/14/14	0/1/1/1
2	MES	F	806	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	F	806	MES	O1S-S-C8	-3.86	103.61	106.91
2	D	804	MES	O1S-S-C8	-2.36	104.89	106.91
2	B	802	MES	O1S-S-C8	-2.32	104.93	106.91
2	A	801	MES	O1S-S-C8	-2.02	105.18	106.91
2	A	801	MES	O2S-S-C8	2.03	108.63	106.91
2	F	806	MES	O2S-S-C8	2.65	109.16	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	MES	1	0
2	C	803	MES	2	0
2	E	805	MES	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	753/772 (97%)	0.35	84 (11%) 7 7	29, 45, 79, 101	0
1	B	741/772 (95%)	0.39	66 (8%) 12 12	31, 45, 86, 102	0
1	C	737/772 (95%)	0.24	45 (6%) 25 25	30, 43, 75, 95	0
1	D	738/772 (95%)	0.25	64 (8%) 13 12	29, 42, 75, 100	0
1	E	736/772 (95%)	0.39	78 (10%) 8 8	31, 47, 79, 99	0
1	F	738/772 (95%)	0.46	78 (10%) 8 8	32, 48, 82, 100	0
All	All	4443/4632 (95%)	0.35	415 (9%) 11 10	29, 45, 79, 102	0

All (415) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	772	LEU	17.8
1	A	516	GLU	11.4
1	B	768	LEU	11.0
1	F	766	ASN	10.4
1	C	287	ASN	10.4
1	F	767	ALA	10.0
1	B	772	LEU	9.9
1	C	518	THR	9.8
1	F	765	GLY	9.8
1	D	765	GLY	9.5
1	F	552	ASP	8.9
1	B	89	ASP	8.8
1	E	484	TYR	8.4
1	B	298	LEU	8.3
1	F	281	TYR	7.9
1	B	389	PHE	7.5
1	B	41	VAL	7.5
1	A	517	ASN	7.4
1	C	300	LEU	7.4

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Mol	Chain	Res	Type	RSRZ
1	D	290	ILE	7.3
1	A	731	ALA	7.1
1	E	765	GLY	7.0
1	E	452	LEU	6.8
1	A	280	ASN	6.7
1	B	88	GLN	6.4
1	F	759	LEU	6.3
1	E	519	ALA	6.3
1	B	767	ALA	6.1
1	A	712	PHE	5.9
1	B	296	ARG	5.9
1	A	286	VAL	5.9
1	B	286	VAL	5.9
1	D	319	GLU	5.8
1	F	656	PHE	5.7
1	A	518	THR	5.7
1	E	766	ASN	5.7
1	F	553	ASP	5.6
1	A	772	LEU	5.6
1	C	297	ASN	5.5
1	F	744	VAL	5.5
1	A	284	ALA	5.4
1	A	745	ASN	5.3
1	D	719	THR	5.3
1	B	302	VAL	5.2
1	E	42	ARG	5.1
1	E	276	SER	5.1
1	F	289	PHE	5.1
1	F	314	GLN	5.0
1	E	767	ALA	5.0
1	A	89	ASP	5.0
1	F	745	ASN	4.9
1	C	770	ILE	4.9
1	B	295	GLU	4.8
1	C	519	ALA	4.8
1	F	706	ALA	4.8
1	D	14	LEU	4.7
1	A	749	ASP	4.7
1	C	276	SER	4.7
1	E	734	TRP	4.6
1	A	14	LEU	4.6
1	B	46	TRP	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	305	PHE	4.6
1	C	720	GLY	4.5
1	D	286	VAL	4.5
1	E	289	PHE	4.5
1	A	48	LEU	4.5
1	A	98	GLU	4.5
1	B	725	VAL	4.4
1	D	724	THR	4.4
1	F	94	ILE	4.4
1	F	738	LEU	4.4
1	F	23	PHE	4.4
1	E	300	LEU	4.4
1	E	485	ALA	4.4
1	E	768	LEU	4.3
1	C	767	ALA	4.3
1	F	521	ALA	4.3
1	A	543	LYS	4.3
1	E	89	ASP	4.2
1	E	108	LEU	4.2
1	D	91	LYS	4.2
1	C	681	VAL	4.2
1	E	290	ILE	4.2
1	F	535	SER	4.2
1	E	278	THR	4.2
1	E	461	ALA	4.1
1	D	552	ASP	4.1
1	E	764	GLN	4.1
1	D	484	TYR	4.1
1	E	772	LEU	4.1
1	B	718	ARG	4.0
1	B	297	ASN	4.0
1	E	320	TRP	4.0
1	A	291	ASP	4.0
1	E	759	LEU	4.0
1	C	733	ASN	4.0
1	C	772	LEU	4.0
1	F	404	GLY	4.0
1	D	721	ASN	3.9
1	D	690	LEU	3.9
1	A	305	PHE	3.9
1	F	315	TRP	3.8
1	C	768	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	46	TRP	3.8
1	D	696	GLY	3.8
1	D	553	ASP	3.8
1	D	729	GLY	3.8
1	A	500	ILE	3.8
1	A	766	ASN	3.8
1	A	711	ILE	3.7
1	D	281	TYR	3.7
1	D	282	ASP	3.7
1	F	286	VAL	3.7
1	E	234	SER	3.7
1	F	736	LEU	3.7
1	F	316	CYS	3.7
1	D	300	LEU	3.7
1	B	695	ASP	3.7
1	F	742	VAL	3.6
1	A	281	TYR	3.6
1	C	275	THR	3.6
1	C	735	THR	3.6
1	B	734	TRP	3.6
1	D	738	LEU	3.6
1	A	393	ASP	3.5
1	B	288	SER	3.5
1	D	534	SER	3.5
1	E	323	LEU	3.5
1	A	734	TRP	3.5
1	C	517	ASN	3.5
1	B	477	VAL	3.5
1	B	657	LEU	3.5
1	B	736	LEU	3.5
1	D	477	VAL	3.5
1	D	659	LEU	3.5
1	F	509	SER	3.5
1	A	732	LYS	3.5
1	B	714	LEU	3.5
1	E	112	VAL	3.4
1	D	394	ALA	3.4
1	C	91	LYS	3.4
1	C	277	PHE	3.4
1	A	501	GLY	3.4
1	E	725	VAL	3.4
1	C	771	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	279	THR	3.4
1	E	44	ARG	3.4
1	C	296	ARG	3.4
1	C	656	PHE	3.4
1	A	290	ILE	3.4
1	D	718	ARG	3.4
1	D	27	GLN	3.3
1	D	764	GLN	3.3
1	B	682	TRP	3.3
1	C	736	LEU	3.3
1	E	76	LEU	3.3
1	F	273	LEU	3.3
1	A	747	LEU	3.3
1	C	298	LEU	3.3
1	E	539	LEU	3.3
1	B	22	VAL	3.3
1	A	285	THR	3.3
1	A	87	LEU	3.3
1	E	744	VAL	3.3
1	B	688	PHE	3.3
1	D	289	PHE	3.3
1	F	290	ILE	3.3
1	A	22	VAL	3.3
1	F	482	ASP	3.3
1	D	695	ASP	3.2
1	D	634	ARG	3.2
1	B	117	PHE	3.2
1	E	714	LEU	3.2
1	B	387	TYR	3.2
1	A	244	GLY	3.2
1	E	277	PHE	3.2
1	F	534	SER	3.2
1	A	46	TRP	3.2
1	D	292	GLY	3.2
1	A	464	PHE	3.2
1	F	464	PHE	3.2
1	C	732	LYS	3.2
1	B	317	ASP	3.2
1	C	46	TRP	3.2
1	A	515	PHE	3.2
1	F	279	THR	3.2
1	D	112	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	738	LEU	3.2
1	E	291	ASP	3.2
1	E	577	ALA	3.2
1	F	729	GLY	3.2
1	A	539	LEU	3.1
1	C	616	VAL	3.1
1	D	535	SER	3.1
1	A	277	PHE	3.1
1	F	465	ALA	3.1
1	E	747	LEU	3.1
1	A	308	PHE	3.1
1	C	608	TYR	3.1
1	B	105	SER	3.1
1	E	456	VAL	3.0
1	C	684	GLU	3.0
1	D	26	GLU	3.0
1	B	515	PHE	3.0
1	B	415	THR	3.0
1	C	652	GLN	3.0
1	E	711	ILE	3.0
1	E	752	GLN	3.0
1	E	296	ARG	3.0
1	D	116	GLU	2.9
1	F	280	ASN	2.9
1	F	760	VAL	2.9
1	A	333	ARG	2.9
1	D	53	PHE	2.9
1	A	717	ALA	2.9
1	F	89	ASP	2.9
1	F	761	VAL	2.9
1	D	374	LEU	2.9
1	D	386	ILE	2.9
1	F	487	TYR	2.9
1	D	464	PHE	2.9
1	A	730	GLU	2.9
1	B	623	ALA	2.9
1	D	454	ASP	2.9
1	E	275	THR	2.9
1	D	497	GLY	2.9
1	C	524	TYR	2.8
1	B	766	ASN	2.8
1	F	244	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	100	TYR	2.8
1	B	43	GLU	2.8
1	B	127	GLU	2.8
1	A	512	ILE	2.8
1	F	681	VAL	2.8
1	F	631	PRO	2.8
1	A	764	GLN	2.8
1	B	319	GLU	2.8
1	E	555	SER	2.8
1	B	244	GLY	2.7
1	B	162	VAL	2.7
1	B	198	PRO	2.7
1	B	305	PHE	2.7
1	E	535	SER	2.7
1	F	197	ILE	2.7
1	A	502	LEU	2.7
1	F	120	LEU	2.7
1	F	484	TYR	2.7
1	C	481	GLY	2.7
1	F	708	GLY	2.7
1	B	303	PHE	2.7
1	B	243	ASP	2.7
1	D	476	PRO	2.7
1	C	730	GLU	2.7
1	A	88	GLN	2.7
1	F	682	TRP	2.7
1	E	79	GLY	2.7
1	A	458	GLU	2.6
1	F	648	ARG	2.6
1	E	476	PRO	2.6
1	F	554	GLU	2.6
1	F	337	ALA	2.6
1	A	145	ASN	2.6
1	F	680	TYR	2.6
1	A	113	SER	2.6
1	B	716	ALA	2.6
1	F	523	VAL	2.6
1	F	91	LYS	2.6
1	B	491	ALA	2.6
1	C	632	GLU	2.6
1	E	634	ARG	2.6
1	A	709	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	52	LEU	2.6
1	B	279	THR	2.6
1	D	143	THR	2.6
1	F	536	HIS	2.6
1	E	558	VAL	2.5
1	F	99	ARG	2.5
1	B	514	GLY	2.5
1	D	728	ALA	2.5
1	F	173	VAL	2.5
1	D	767	ALA	2.5
1	A	708	GLY	2.5
1	C	477	VAL	2.5
1	E	760	VAL	2.5
1	F	731	ALA	2.5
1	F	22	VAL	2.5
1	F	92	VAL	2.5
1	B	42	ARG	2.5
1	D	770	ILE	2.5
1	E	303	PHE	2.5
1	E	235	GLU	2.5
1	F	520	PRO	2.5
1	A	729	GLY	2.5
1	C	398	TYR	2.5
1	D	633	GLY	2.5
1	F	613	ASN	2.5
1	A	509	SER	2.5
1	B	299	PRO	2.4
1	E	477	VAL	2.4
1	E	301	HIS	2.4
1	F	508	TRP	2.4
1	A	738	LEU	2.4
1	F	610	LEU	2.4
1	F	414	LYS	2.4
1	E	333	ARG	2.4
1	A	118	TRP	2.4
1	E	273	LEU	2.4
1	A	287	ASN	2.4
1	E	397	TRP	2.4
1	A	414	LYS	2.4
1	A	503	SER	2.4
1	D	89	ASP	2.4
1	A	697	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	288	SER	2.4
1	F	477	VAL	2.4
1	A	662	TYR	2.4
1	C	766	ASN	2.4
1	C	173	VAL	2.4
1	D	703	VAL	2.4
1	C	98	GLU	2.4
1	D	524	TYR	2.4
1	F	505	PHE	2.4
1	C	92	VAL	2.4
1	E	334	ARG	2.4
1	A	723	ILE	2.4
1	E	3	ILE	2.4
1	A	343	CYS	2.3
1	E	684	GLU	2.3
1	D	536	HIS	2.3
1	F	166	GLY	2.3
1	A	345	TRP	2.3
1	F	533	LEU	2.3
1	E	299	PRO	2.3
1	B	508	TRP	2.3
1	F	368	LYS	2.3
1	A	283	GLU	2.3
1	C	695	ASP	2.3
1	D	617	ALA	2.3
1	D	723	ILE	2.3
1	E	58	PHE	2.3
1	A	47	GLN	2.3
1	A	346	ILE	2.3
1	E	363	LYS	2.3
1	A	166	GLY	2.3
1	D	682	TRP	2.3
1	F	752	GLN	2.3
1	F	747	LEU	2.3
1	F	291	ASP	2.3
1	A	208	VAL	2.3
1	F	344	VAL	2.3
1	B	413	PHE	2.2
1	B	505	PHE	2.2
1	B	454	ASP	2.2
1	E	166	GLY	2.2
1	B	698	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	756	GLU	2.2
1	D	648	ARG	2.2
1	A	342	ILE	2.2
1	E	49	ASP	2.2
1	B	556	CYS	2.2
1	A	548	PRO	2.2
1	A	761	VAL	2.2
1	A	99	ARG	2.2
1	A	428	PHE	2.2
1	E	365	TYR	2.2
1	E	761	VAL	2.2
1	E	625	ASP	2.2
1	B	464	PHE	2.2
1	F	269	PHE	2.2
1	B	281	TYR	2.2
1	B	445	ASN	2.2
1	C	701	CYS	2.2
1	C	26	GLU	2.2
1	D	366	LEU	2.2
1	E	41	VAL	2.2
1	B	467	SER	2.2
1	E	534	SER	2.2
1	F	577	ALA	2.2
1	F	285	THR	2.2
1	A	540	HIS	2.1
1	A	499	SER	2.1
1	F	105	SER	2.1
1	A	427	TRP	2.1
1	D	635	TRP	2.1
1	A	100	TYR	2.1
1	A	714	LEU	2.1
1	B	405	LEU	2.1
1	E	316	CYS	2.1
1	F	476	PRO	2.1
1	A	157	GLY	2.1
1	C	718	ARG	2.1
1	A	552	ASP	2.1
1	A	423	THR	2.1
1	A	332	ILE	2.1
1	B	463	LEU	2.1
1	E	40	ASP	2.1
1	B	534	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	479	TRP	2.1
1	D	453	LYS	2.1
1	E	247	PRO	2.1
1	E	264	PRO	2.1
1	E	144	ASN	2.0
1	E	716	ALA	2.0
1	B	122	PHE	2.0
1	D	308	PHE	2.0
1	B	388	ASP	2.0
1	A	165	LEU	2.0
1	D	720	GLY	2.0
1	D	761	VAL	2.0
1	F	106	GLY	2.0
1	E	127	GLU	2.0
1	E	627	GLN	2.0
1	C	76	LEU	2.0
1	A	320	TRP	2.0
1	D	303	PHE	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MES	B	802	12/12	0.91	0.27	1.05	81,85,86,87	0
2	MES	F	806	12/12	0.92	0.24	0.63	67,73,76,76	0
2	MES	A	801	12/12	0.85	0.30	0.60	81,82,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MES	E	805	12/12	0.84	0.25	0.58	79,80,81,81	0
2	MES	C	803	12/12	0.84	0.24	0.20	54,59,60,62	0
2	MES	D	804	12/12	0.97	0.10	-1.03	56,64,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.