



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:53 AM UTC

PDB ID : 1WE5 / pdb_00001we5
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

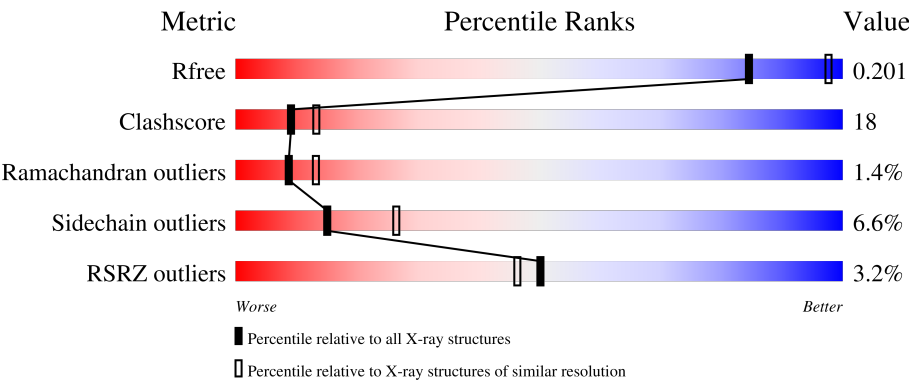
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	772	3% 66%29%.
1	B	772	4% 63%30%5%..
1	C	772	3% 62%29%5%..
1	D	772	2% 63%30%5%.
1	E	772	4% 62%31%5%.

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Mol	Chain	Length	Quality of chain
1	F	772	3% 66% 27%

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
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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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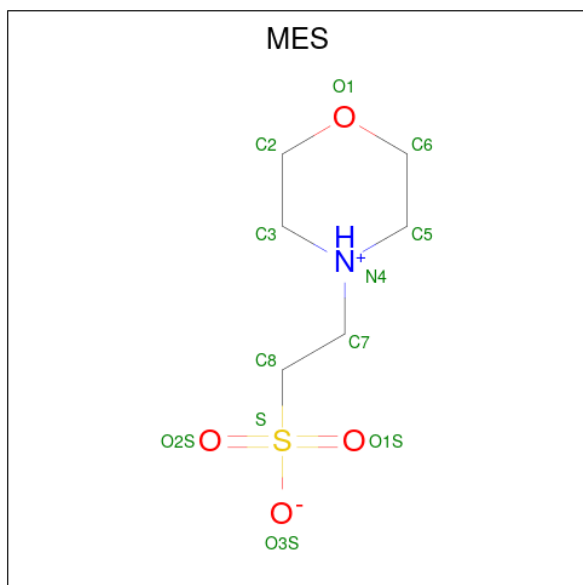
Chain	Residue	Modelled	Actual	Comment	Reference
D	150	MSE	MET	modified residue	UNP P31434
D	201	MSE	MET	modified residue	UNP P31434
D	293	MSE	MET	modified residue	UNP P31434
D	310	MSE	MET	modified residue	UNP P31434
D	331	MSE	MET	modified residue	UNP P31434
D	408	MSE	MET	modified residue	UNP P31434
D	436	MSE	MET	modified residue	UNP P31434
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D	569	MSE	MET	modified residue	UNP P31434
D	570	MSE	MET	modified residue	UNP P31434
D	587	MSE	MET	modified residue	UNP P31434
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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
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E	310	MSE	MET	modified residue	UNP P31434
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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 (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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		

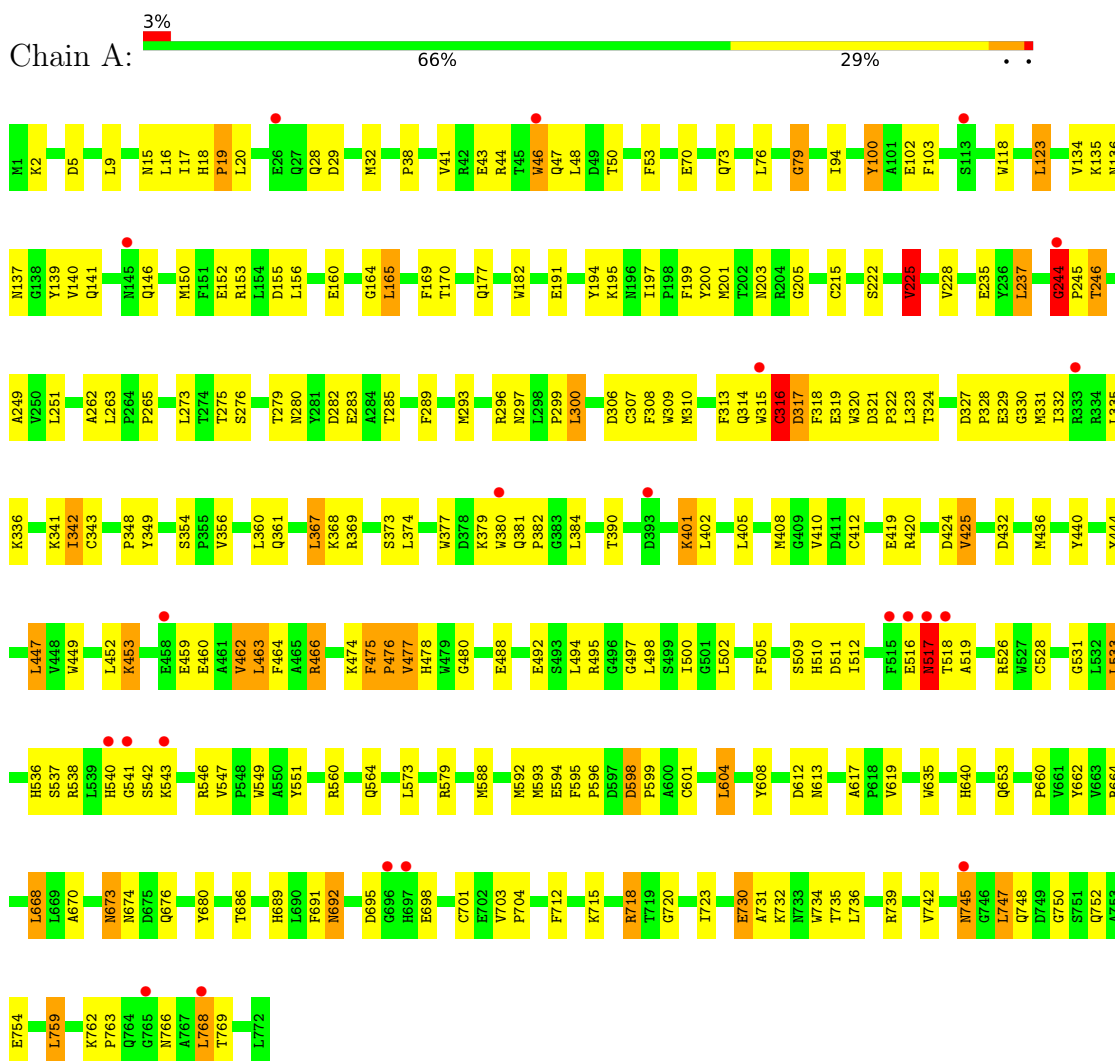
- Molecule 3 is water.

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		

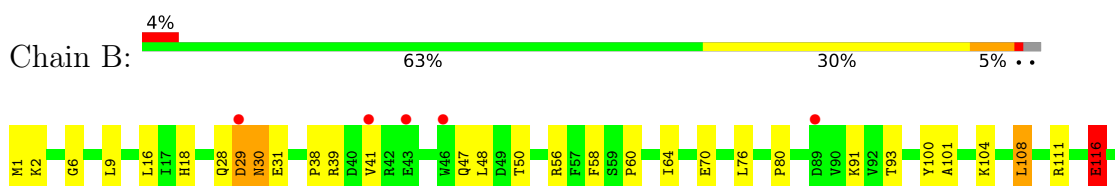
3 Residue-property plots [i](#)

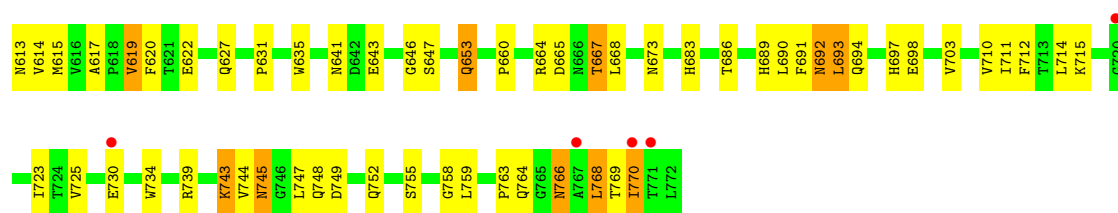
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Putative family 31 glucosidase yicI

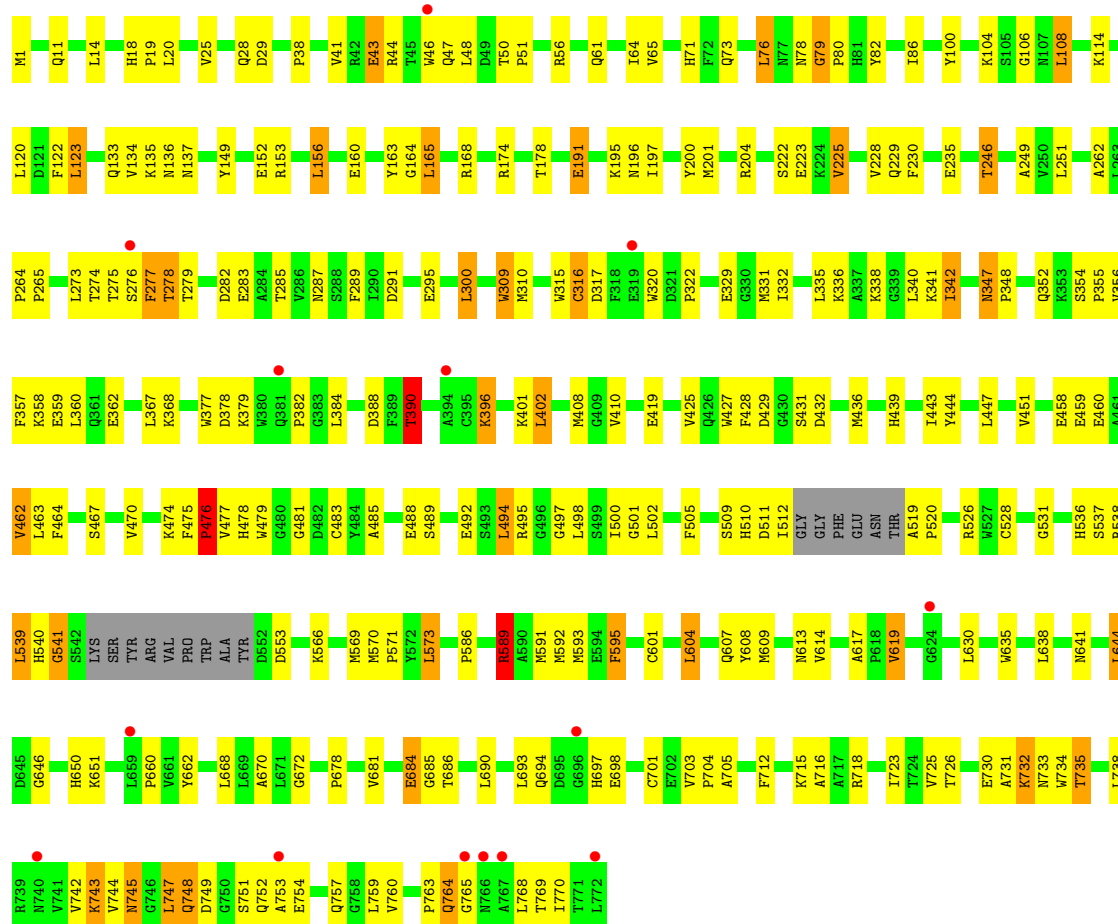


• Molecule 1: Putative family 31 glucosidase yicI

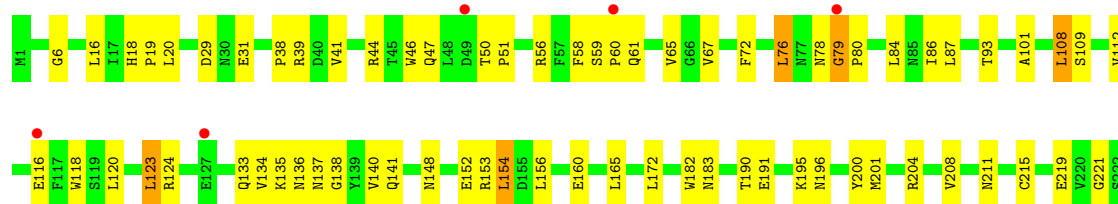


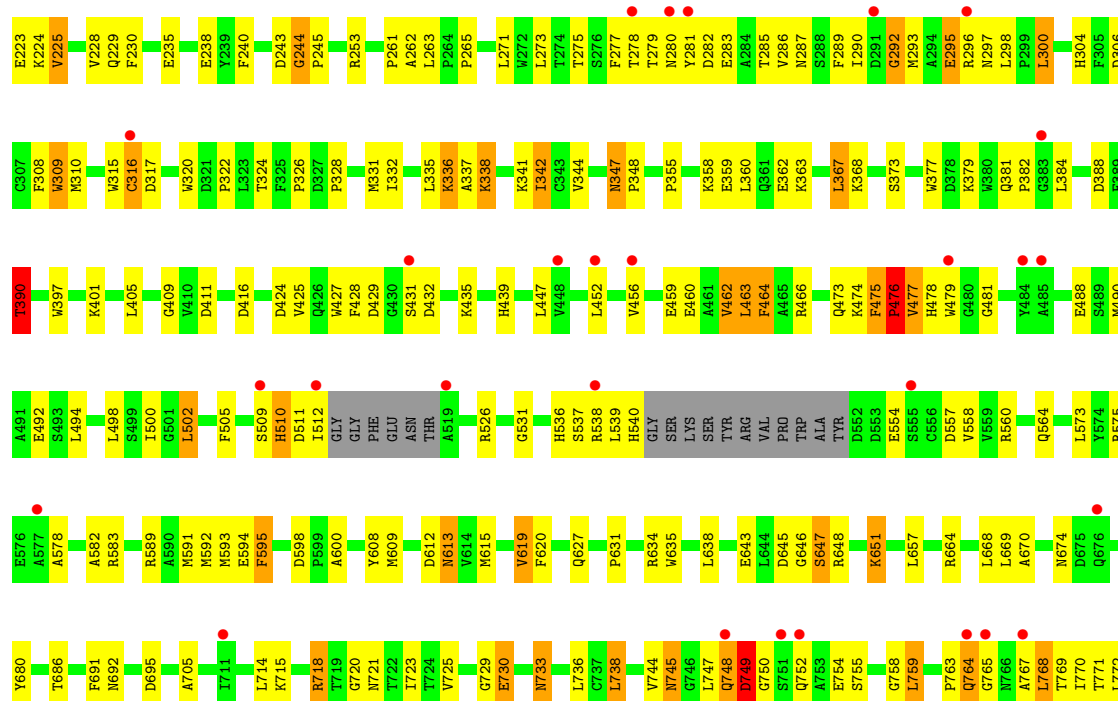


• Molecule 1: Putative family 31 glucosidase yicI

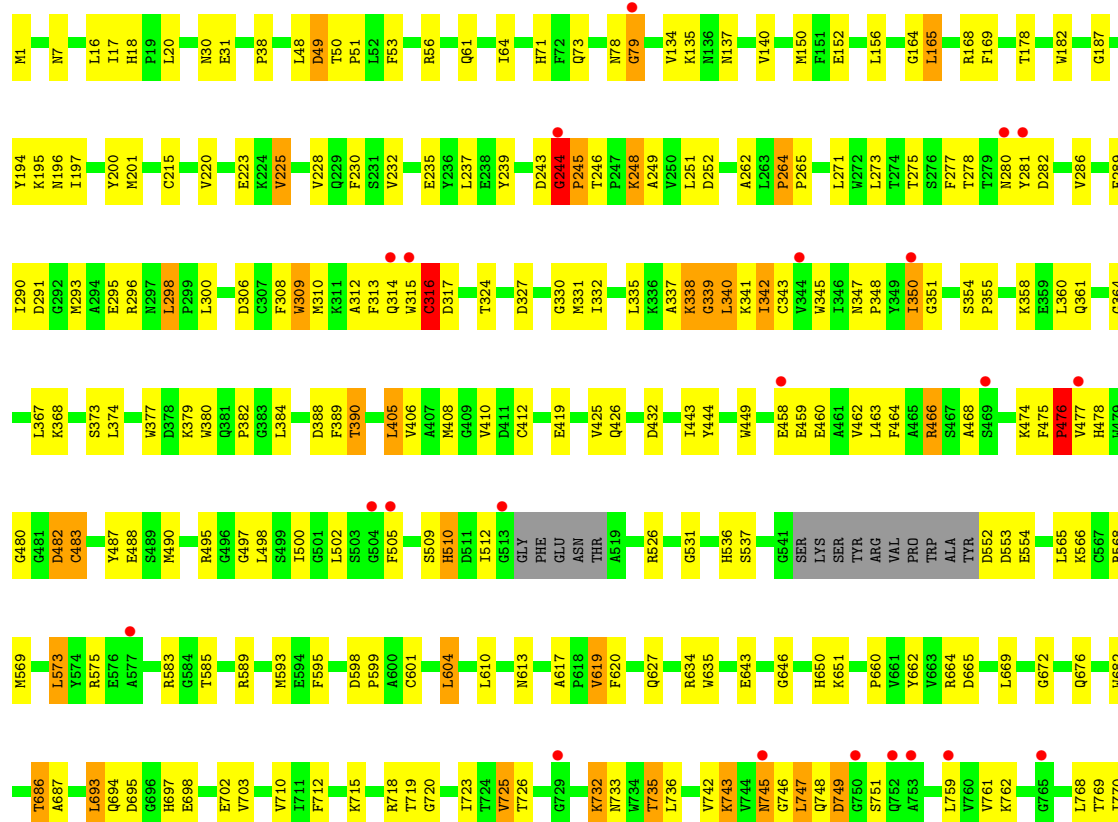


• Molecule 1: Putative family 31 glucosidase yicI





• 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 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (15.00-2.40) 98.8 (15.00-2.40)	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	20756 reflections (9.07%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 12.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	0/6387	0.96	24/8650 (0.3%)
1	B	0.42	0/6280	0.98	38/8502 (0.4%)
1	C	0.43	0/6250	0.98	32/8461 (0.4%)
1	D	0.43	0/6253	0.98	25/8464 (0.3%)
1	E	0.41	0/6243	0.96	32/8451 (0.4%)
1	F	0.40	0/6251	0.94	23/8461 (0.3%)
All	All	0.42	0/37664	0.97	174/50989 (0.3%)

There are no bond length outliers.

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	416	ASP	N-CA-C	12.74	127.36	111.69
1	F	475	PHE	CA-C-N	11.38	134.07	119.84
1	F	475	PHE	C-N-CA	11.38	134.07	119.84
1	B	416	ASP	N-CA-C	10.86	126.36	112.89
1	D	279	THR	N-CA-C	10.68	125.69	112.87
1	A	317	ASP	N-CA-C	-10.10	98.70	112.94
1	D	475	PHE	CA-C-N	10.02	132.36	119.84
1	D	475	PHE	C-N-CA	10.02	132.36	119.84
1	C	475	PHE	CA-C-N	9.72	131.99	119.84
1	C	475	PHE	C-N-CA	9.72	131.99	119.84
1	E	475	PHE	CA-C-N	9.54	131.77	119.84
1	E	475	PHE	C-N-CA	9.54	131.77	119.84
1	A	475	PHE	CA-C-N	9.47	131.68	119.84
1	A	475	PHE	C-N-CA	9.47	131.68	119.84
1	D	613	ASN	N-CA-C	8.95	125.36	113.72
1	F	317	ASP	N-CA-C	-8.78	100.44	113.61
1	E	317	ASP	N-CA-C	-8.59	100.82	112.94
1	B	475	PHE	CA-C-N	8.51	130.47	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	475	PHE	C-N-CA	8.51	130.47	119.84
1	B	223	GLU	N-CA-C	-8.19	101.14	112.12
1	E	223	GLU	N-CA-C	-8.02	101.37	112.12
1	B	317	ASP	N-CA-C	-7.78	102.88	113.30
1	B	764	GLN	N-CA-C	-7.76	104.74	112.97
1	C	317	ASP	N-CA-C	-7.72	102.95	113.30
1	D	309	TRP	N-CA-C	-7.71	103.86	113.18
1	D	317	ASP	N-CA-C	-7.70	102.98	113.30
1	F	337	ALA	N-CA-C	-7.57	103.03	111.28
1	E	295	GLU	N-CA-C	-7.50	100.86	110.53
1	C	223	GLU	N-CA-C	-7.41	102.19	112.12
1	E	613	ASN	N-CA-C	7.36	121.97	112.41
1	F	315	TRP	N-CA-C	7.34	120.90	109.96
1	B	379	LYS	N-CA-C	7.33	119.91	111.11
1	A	613	ASN	N-CA-C	7.30	123.08	113.30
1	C	315	TRP	N-CA-C	7.06	120.88	110.30
1	E	764	GLN	N-CA-C	-7.00	102.73	112.25
1	B	30	ASN	N-CA-C	-6.96	104.37	112.92
1	D	390	THR	N-CA-C	-6.93	104.85	113.38
1	B	164	GLY	N-CA-C	6.93	119.97	111.45
1	B	309	TRP	N-CA-C	-6.89	104.73	113.01
1	E	315	TRP	N-CA-C	6.84	120.76	110.64
1	F	613	ASN	N-CA-C	6.84	122.58	112.94
1	C	612	ASP	N-CA-C	6.78	118.67	111.28
1	E	612	ASP	N-CA-C	6.73	118.61	111.28
1	D	315	TRP	N-CA-C	6.69	120.34	110.30
1	A	595	PHE	CA-C-N	6.66	126.61	119.28
1	A	595	PHE	C-N-CA	6.66	126.61	119.28
1	F	309	TRP	N-CA-C	-6.62	105.16	113.18
1	D	278	THR	N-CA-C	6.62	119.50	111.82
1	E	309	TRP	N-CA-C	-6.62	105.17	113.18
1	B	595	PHE	CA-C-N	6.55	126.32	119.05
1	B	595	PHE	C-N-CA	6.55	126.32	119.05
1	C	613	ASN	N-CA-C	6.54	123.42	113.61
1	D	225	VAL	N-CA-C	6.49	120.13	111.17
1	F	225	VAL	N-CA-C	6.47	120.10	111.17
1	B	613	ASN	N-CA-C	6.46	123.30	113.61
1	F	244	GLY	N-CA-C	-6.38	99.34	112.34
1	E	341	LYS	N-CA-C	-6.32	100.00	110.17
1	E	390	THR	N-CA-C	-6.27	105.56	113.72
1	C	45	THR	N-CA-C	-6.27	102.26	110.53
1	A	244	GLY	N-CA-C	-6.26	99.58	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	390	THR	N-CA-C	-6.14	105.82	113.38
1	E	336	LYS	N-CA-C	-6.14	100.21	109.60
1	C	70	GLU	N-CA-C	6.14	119.54	109.72
1	D	341	LYS	N-CA-C	-6.13	100.29	110.17
1	F	476	PRO	N-CA-C	6.12	125.09	112.47
1	B	725	VAL	N-CA-C	6.12	112.76	106.21
1	E	244	GLY	N-CA-C	-6.08	99.93	112.34
1	F	178	THR	N-CA-C	-6.06	99.82	109.76
1	B	612	ASP	N-CA-C	6.04	117.87	111.28
1	E	595	PHE	CA-C-N	6.04	125.72	119.56
1	E	595	PHE	C-N-CA	6.04	125.72	119.56
1	D	315	TRP	CA-C-N	6.03	133.05	121.54
1	D	315	TRP	C-N-CA	6.03	133.05	121.54
1	A	369	ARG	N-CA-C	-6.02	102.29	110.36
1	B	101	ALA	N-CA-C	-5.97	97.40	108.02
1	F	595	PHE	CA-C-N	5.96	126.11	119.32
1	F	595	PHE	C-N-CA	5.96	126.11	119.32
1	E	211	ASN	N-CA-C	5.95	118.85	109.39
1	B	244	GLY	N-CA-C	-5.93	100.24	112.34
1	C	485	ALA	N-CA-C	5.91	119.85	110.70
1	D	595	PHE	CA-C-N	5.90	126.31	119.47
1	D	595	PHE	C-N-CA	5.90	126.31	119.47
1	D	164	GLY	N-CA-C	5.89	118.69	111.45
1	B	485	ALA	N-CA-C	5.89	118.01	109.71
1	C	315	TRP	CA-C-N	5.88	132.77	121.54
1	C	315	TRP	C-N-CA	5.88	132.77	121.54
1	B	390	THR	N-CA-C	-5.87	106.16	113.38
1	B	646	GLY	N-CA-C	5.87	121.22	112.41
1	A	315	TRP	N-CA-C	5.85	118.19	109.59
1	A	390	THR	N-CA-C	-5.83	105.83	113.17
1	B	174	ARG	N-CA-C	5.82	119.63	112.54
1	C	244	GLY	N-CA-C	-5.81	100.49	112.34
1	A	730	GLU	N-CA-C	5.81	118.68	108.75
1	C	101	ALA	N-CA-C	-5.78	98.99	108.41
1	D	705	ALA	N-CA-C	-5.76	102.23	110.59
1	F	342	ILE	N-CA-C	5.76	116.78	108.48
1	E	6	GLY	N-CA-C	-5.75	102.23	112.58
1	A	19	PRO	N-CA-C	-5.73	100.81	110.21
1	E	476	PRO	N-CA-C	5.73	124.28	112.47
1	A	598	ASP	CA-C-N	5.73	125.58	119.28
1	A	598	ASP	C-N-CA	5.73	125.58	119.28
1	F	390	THR	N-CA-C	-5.70	106.37	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	342	ILE	N-CA-C	5.69	116.07	108.11
1	E	589	ARG	N-CA-C	5.62	118.11	109.07
1	A	164	GLY	N-CA-C	5.61	118.34	111.45
1	C	327	ASP	CA-C-N	5.60	125.06	119.24
1	C	327	ASP	C-N-CA	5.60	125.06	119.24
1	C	47	GLN	N-CA-C	-5.59	103.89	111.55
1	F	264	PRO	CA-C-N	5.57	125.75	119.90
1	F	264	PRO	C-N-CA	5.57	125.75	119.90
1	B	391	ASN	CA-C-N	5.55	125.01	119.24
1	B	391	ASN	C-N-CA	5.55	125.01	119.24
1	D	646	GLY	N-CA-C	5.55	120.73	112.41
1	B	315	TRP	N-CA-C	5.54	118.61	110.30
1	A	640	HIS	N-CA-C	-5.47	106.45	113.23
1	E	598	ASP	CA-C-N	5.46	125.80	119.47
1	E	598	ASP	C-N-CA	5.46	125.80	119.47
1	A	612	ASP	N-CA-C	5.44	117.29	111.36
1	F	589	ARG	N-CA-C	5.42	117.80	109.07
1	E	292	GLY	N-CA-C	-5.42	106.11	113.37
1	C	309	TRP	N-CA-C	-5.40	106.53	113.01
1	D	19	PRO	N-CA-C	-5.38	101.81	110.74
1	E	225	VAL	N-CA-C	5.38	118.60	111.17
1	C	263	LEU	CA-C-N	5.38	123.53	119.66
1	C	263	LEU	C-N-CA	5.38	123.53	119.66
1	A	341	LYS	N-CA-C	-5.37	101.41	109.95
1	C	308	PHE	N-CA-C	5.34	120.75	113.37
1	D	100	TYR	N-CA-C	5.34	117.53	109.41
1	D	86	ILE	N-CA-C	5.34	114.43	106.85
1	A	480	GLY	N-CA-C	5.33	121.92	115.31
1	D	178	THR	N-CA-C	-5.30	100.54	109.07
1	A	424	ASP	N-CA-C	-5.29	103.33	110.68
1	B	279	THR	N-CA-C	5.29	119.60	113.20
1	C	539	LEU	N-CA-C	5.28	117.84	111.40
1	F	646	GLY	N-CA-C	5.28	120.33	112.41
1	C	341	LYS	N-CA-C	-5.28	101.93	110.32
1	E	705	ALA	N-CA-C	-5.27	102.66	110.46
1	A	155	ASP	N-CA-C	5.26	117.50	110.35
1	F	338	LYS	N-CA-C	-5.24	101.99	110.32
1	A	225	VAL	N-CA-C	5.24	118.40	111.17
1	E	86	ILE	N-CA-C	5.24	115.12	107.37
1	B	211	ASN	N-CA-C	5.23	118.81	110.70
1	B	6	GLY	N-CA-C	-5.23	103.31	112.77
1	F	340	LEU	N-CA-C	5.23	121.94	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	ARG	N-CA-C	-5.21	105.28	111.69
1	B	116	GLU	N-CA-C	5.21	117.70	111.71
1	B	315	TRP	CA-C-N	5.20	131.47	121.54
1	B	315	TRP	C-N-CA	5.20	131.47	121.54
1	C	589	ARG	N-CA-C	5.20	117.96	109.59
1	C	614	VAL	N-CA-C	5.20	115.34	107.75
1	D	614	VAL	N-CA-C	5.20	115.44	108.17
1	E	315	TRP	CA-C-N	5.19	131.45	121.54
1	E	315	TRP	C-N-CA	5.19	131.45	121.54
1	B	225	VAL	N-CA-C	5.16	120.07	109.34
1	B	293	MSE	N-CA-C	-5.16	107.12	113.41
1	C	575	ARG	N-CA-C	-5.15	105.74	111.36
1	C	476	PRO	N-CA-C	5.15	123.07	112.47
1	B	70	GLU	N-CA-C	5.14	117.94	109.72
1	E	19	PRO	N-CA-C	-5.14	101.89	112.47
1	E	138	GLY	N-CA-C	5.14	116.95	110.38
1	B	316	CYS	CA-CB-SG	-5.10	102.66	114.40
1	D	223	GLU	N-CA-C	-5.10	105.14	112.13
1	A	342	ILE	N-CA-C	5.08	115.80	108.48
1	A	100	TYR	N-CA-C	5.07	116.00	108.60
1	F	480	GLY	N-CA-C	5.06	119.87	113.24
1	C	138	GLY	N-CA-C	5.06	116.85	110.38
1	B	342	ILE	N-CA-C	5.03	115.16	108.11
1	D	589	ARG	N-CA-C	5.03	118.01	109.76
1	C	764	GLN	N-CA-C	-5.03	101.45	108.54
1	B	563	THR	N-CA-C	-5.02	105.89	111.36
1	B	589	ARG	N-CA-C	5.02	117.67	109.59
1	E	424	ASP	N-CA-C	-5.01	103.72	110.68
1	F	487	TYR	N-CA-C	5.01	116.74	111.28
1	E	647	SER	N-CA-C	-5.01	107.12	113.23

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	246	0
1	B	6121	0	5839	235	0
1	C	6093	0	5817	239	0
1	D	6096	0	5816	210	0
1	E	6086	0	5808	235	0
1	F	6094	0	5814	200	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	1317	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 (1317) 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:H	1:B:358:LYS:HD2	1.08	1.06
1:B:690:LEU:HD11	1:B:693:LEU:HB2	1.31	1.05
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD2	1:B:358:LYS:N	1.86	0.89
1:E:609:MSE:HE1	1:E:615:MSE:CG	2.02	0.89
1:C:591:MSE:HE1	1:C:615:MSE:HG2	1.53	0.89
1:D:690:LEU:HD11	1:D:693:LEU:HB2	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:332:ILE:HD12	1:F:408:MSE:HE2	1.58	0.84
1:F:526:ARG:HD2	1:F:619:VAL:HG22	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:A:332:ILE:HD12	1:A:408:MSE:HE2	1.59	0.83
1:B:668:LEU:HD13	1:B:690:LEU:HD23	1.60	0.83
1:A:488:GLU:O	1:A:492:GLU:HG3	1.78	0.82
1:D:246:THR:HG22	1:D:249:ALA:H	1.44	0.82
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:D:388:ASP:OD1	1:D:390:THR:HG22	1.81	0.80
1:E:609:MSE:CE	1:E:615:MSE:HG2	2.11	0.80
1:E:526:ARG:HD2	1:E:619:VAL:HG22	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:31:GLU:HG2	1:C:58:PHE:HB3	1.64	0.79
1:D:595:PHE:CE1	1:D:609:MSE:HE3	2.17	0.79
1:E:609:MSE:CE	1:E:615:MSE:HA	2.13	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:B:474:LYS:C	1:B:476:PRO:HD3	2.08	0.78
1:A:763:PRO:HB3	1:A:768:LEU:HD12	1.66	0.77
1:D:748:GLN:HB2	1:D:769:THR:HG22	1.66	0.77
1:A:32:MSE:HE2	1:A:94:ILE:CG2	2.10	0.77
1:A:44:ARG:HH21	1:C:278:THR:HA	1.47	0.77
1:B:300:LEU:HD13	1:B:340:LEU:HD21	1.66	0.77
1:E:282:ASP:O	1:E:285:THR:HG22	1.83	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:A:314:GLN:HB2	1:A:354:SER:HB2	1.66	0.77
1:D:595:PHE:HE1	1:D:609:MSE:HE3	1.49	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:C:44:ARG:O	1:C:47:GLN:HB2	1.86	0.76
1:E:342:ILE:H	1:E:342:ILE:HD13	1.51	0.76
1:F:314:GLN:HB2	1:F:354:SER:HB2	1.67	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:ASN:C	1:E:347:ASN:HD22	1.96	0.74
1:A:32:MSE:HE1	1:A:102:GLU:O	1.87	0.74
1:B:711:ILE:H	1:B:711:ILE:HD13	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:474:LYS:C	1:F:476:PRO:HD3	2.12	0.73
1:F:732:LYS:HE2	1:F:732:LYS:HA	1.68	0.73
1:C:88:GLN:CD	1:C:88:GLN:H	1.95	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:A:516:GLU:CD	1:A:516:GLU:H	1.97	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:D:474:LYS:C	1:D:476:PRO:HD3	2.15	0.72
1:D:79:GLY:CA	1:D:432:ASP:H	2.02	0.71
1:E:474:LYS:C	1:E:476:PRO:HD3	2.15	0.71
1:F:566:LYS:HA	1:F:569:MSE:HE3	1.71	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: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:E:714:LEU:HD21	1:E:725:VAL:HG13	1.72	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:B:772:LEU:H	1:B:772:LEU:HD22	1.57	0.70
1:C:703:VAL:CG1	1:C:712:PHE:HB3	2.21	0.70
1:B:314:GLN:HB2	1:B:354:SER:HB2	1.73	0.69

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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: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:F:262:ALA:HB3	1:F:476:PRO:HG2	1.73	0.69
1:F:310:MSE:SE	1:F:316:CYS:HA	2.43	0.69
1:F:474:LYS:O	1:F:476:PRO:HD3	1.92	0.69
1:A:310:MSE:SE	1:A:316:CYS:HA	2.43	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:46:TRP:HA	1:C:46:TRP:CE3	2.27	0.69
1:A:592:MSE:HE3	1:A:593:MSE:CB	2.22	0.68
1:D:526:ARG:HD2	1:D:619:VAL:HG22	1.75	0.68
1:E:295:GLU:O	1:E:296:ARG:HB2	1.93	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:B:29:ASP:CG	1:B:30:ASN:H	2.01	0.68
1:A:331:MSE:O	1:A:335:LEU:HD13	1.94	0.68
1:A:474:LYS:C	1:A:476:PRO:HD3	2.18	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:B:100:TYR:CD2	1:B:111:ARG:HD3	2.29	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:F:725:VAL:HG13	1:F:768:LEU:HB3	1.76	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: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: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:425:VAL:CG1	1:F:426:GLN:N	2.57	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: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
1:E:44:ARG:HA	1:E:47:GLN:HG3	1.77	0.67
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:C:502:LEU:HD21	1:C:592:MSE:HE1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:425:VAL:HG12	1:F:426:GLN:N	2.09	0.67
1:D:310:MSE:SE	1:D:316:CYS:HA	2.44	0.67
1:E:41:VAL:HG22	1:E:47:GLN:HG2	1.76	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:168:ARG:NH2	1:F:196:ASN:OD1	2.27	0.66
1:F:367:LEU:HD11	1:F:425:VAL:HG11	1.76	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:F:20:LEU:HD12	1:F:38:PRO:O	1.94	0.66
1:B:297:ASN:C	1:B:299:PRO:HD3	2.20	0.66
1:B:690:LEU:CD1	1:B:693:LEU:HB2	2.20	0.66
1:B:474:LYS:O	1:B:476:PRO:HD3	1.95	0.66
1:C:169:PHE:O	1:F:225:VAL:HG11	1.96	0.66
1:D:195:LYS:HE2	1:D:478:HIS:HB3	1.77	0.66
1:D:748:GLN:CB	1:D:769:THR:HG22	2.25	0.66
1:F:150:MSE:HE3	1:F:235:GLU:C	2.20	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:A:79:GLY:CA	1:A:432:ASP:H	2.10	0.65
1:E:367:LEU:HD22	1:E:425:VAL:HG21	1.78	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: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:D:747:LEU:HD12	1:D:748:GLN:H	1.60	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:A:32:MSE:HE1	1:A:102:GLU:C	2.22	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:C:474:LYS:C	1:C:476:PRO:HD3	2.22	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:C:591:MSE:HE2	1:C:608:TYR:CA	2.26	0.64
1:E:608:TYR:O	1:E:609:MSE:HE2	1.98	0.64
1:B:571:PRO:HG3	1:B:682:TRP:CB	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:382:PRO:HG3	1:D:50:THR:O	1.97	0.64
1:B:591:MSE:HE1	1:B:608:TYR:N	2.13	0.64
1:C:388:ASP:OD1	1:C:390:THR:HG22	1.98	0.64
1:E:750:GLY:CA	1:E:764:GLN:HG2	2.28	0.64
1:A:150:MSE:HE3	1:A:235:GLU:C	2.22	0.64
1:E:331:MSE:O	1:E:335:LEU:HD23	1.97	0.64
1:A:731:ALA:C	1:A:732:LYS:HD2	2.22	0.64
1:C:244:GLY:O	1:C:245:PRO:C	2.40	0.64
1:C:46:TRP:HA	1:C:46:TRP:HE3	1.63	0.64
1:C:698:GLU:CD	1:C:715:LYS:HD3	2.23	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:A:244:GLY:O	1:A:245:PRO:C	2.42	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:A:463:LEU:O	1:A:477:VAL:HB	1.99	0.62
1:C:16:LEU:HD22	1:C:140:VAL:HG22	1.81	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:C:522:HIS:CD2	1:C:622:GLU:HB2	2.35	0.62
1:E:763:PRO:HB2	1:E:765:GLY:O	1.98	0.62
1:F:278:THR:HG22	1:F:308:PHE:CE1	2.34	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:766:ASN:C	1:C:766:ASN:HD22	2.08	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:F:296:ARG:HH12	1:F:553:ASP:CG	2.07	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:C:27:GLN:HG3	1:C:94:ILE:CD1	2.30	0.61
1:D:20:LEU:HD11	3:D:1129:HOH:O	1.99	0.61
1:A:698:GLU:CD	1:A:715:LYS:HE2	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:474:LYS:O	1:D:476:PRO:HD3	1.99	0.61
1:E:31:GLU:OE1	1:E:56:ARG:HD3	2.00	0.61
1:E:243:ASP:CG	1:E:244:GLY:H	2.07	0.61
1:E:609:MSE:HE1	1:E:615:MSE:HA	1.81	0.61
1:F:693:LEU:HD13	1:F:718:ARG:HB2	1.81	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: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:D:354:SER:OG	1:D:356:VAL:HG12	2.00	0.61
1:E:560:ARG:O	1:E:564:GLN:HG3	2.01	0.61
1:A:16:LEU:HD22	1:A:140:VAL:HG22	1.82	0.61
1:C:456:VAL:HG12	1:C:460:GLU:CB	2.30	0.61
1:D:347:ASN:C	1:D:347:ASN:HD22	2.08	0.61
1:E:328:PRO:O	1:E:332:ILE:HD13	2.00	0.61
1:B:711:ILE:HG12	1:B:712:PHE:N	2.15	0.61
1:C:282:ASP:H	1:C:285:THR:CG2	2.13	0.61
1:C:41:VAL:HG22	1:C:47:GLN:HG3	1.81	0.60
1:C:484:TYR:HD2	1:C:486:ASN:ND2	1.99	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:8:TRP:C	1:C:9:LEU:HD12	2.26	0.60
1:B:539:LEU:O	1:B:540:HIS:HB3	2.01	0.60
1:C:269:PHE:CE2	1:C:587:MSE:HE1	2.36	0.60
1:B:41:VAL:HG12	1:B:47:GLN:HG2	1.83	0.60
1:B:290:ILE:HG13	1:B:340:LEU:HD11	1.83	0.60
1:E:390:THR:CG2	1:E:429:ASP:H	2.14	0.60
1:F:703:VAL:CG2	1:F:712:PHE:HB3	2.30	0.60
1:B:447:LEU:HD23	1:B:447:LEU:C	2.26	0.60
1:B:638:LEU:HD12	1:B:639:TRP:HE3	1.66	0.60
1:D:246:THR:CG2	1:D:249:ALA:H	2.14	0.60
1:B:641:ASN:HD22	1:B:757:GLN:CG	2.15	0.60
1:C:283:GLU:HA	1:C:331:MSE:CE	2.30	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:E:609:MSE:HE2	1:E:609:MSE:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:LYS:HD2	1:F:585:THR:HG23	1.82	0.60
1:F:698:GLU:OE1	1:F:715:LYS:HD3	2.02	0.60
1:B:497:GLY:O	1:B:500:ILE:HG22	2.02	0.60
1:C:61:GLN:HA	1:C:90:VAL:HG21	1.84	0.60
1:C:694:GLN:HB2	1:C:697:HIS:CD2	2.37	0.60
1:D:512:ILE:HD11	1:D:531:GLY:HA3	1.84	0.60
1:A:41:VAL:HG22	1:A:47:GLN:HG2	1.83	0.60
1:E:347:ASN:C	1:E:347:ASN:ND2	2.58	0.60
1:A:205:GLY:O	1:A:244:GLY:O	2.20	0.60
1:B:1:MSE:HE1	1:B:149:TYR:CZ	2.37	0.60
1:C:485:ALA:HB1	1:C:519:ALA:CB	2.32	0.60
1:E:342:ILE:HD11	1:E:409:GLY:O	2.02	0.60
1:A:32:MSE:HE3	1:A:103:PHE:HB2	1.83	0.59
1:E:295:GLU:C	1:E:297:ASN:H	2.08	0.59
1:A:511:ASP:OD1	1:A:540:HIS:HD2	1.85	0.59
1:B:744:VAL:HG13	1:B:772:LEU:HA	1.84	0.59
1:E:738:LEU:H	1:E:738:LEU:HD22	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:N	1:C:123:LEU:HD22	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: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:273:LEU:HD22	1:E:300:LEU:HD21	1.84	0.59
1:E:750:GLY:HA2	1:E:764:GLN:HG2	1.83	0.59
1:A:689:HIS:CD2	1:A:739:ARG:HH11	2.21	0.59
1:C:485:ALA:HB1	1:C:519:ALA:HB2	1.84	0.59
1:D:591:MSE:HE3	1:D:607:GLN:CG	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:A:297:ASN:O	1:A:299:PRO:HD3	2.02	0.59
1:E:283:GLU:CA	1:E:331:MSE:HE3	2.19	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:B:601:CYS:HA	1:B:604:LEU:HD22	1.85	0.59
1:C:290:ILE:HD11	1:C:338:LYS:HD2	1.84	0.59
1:C:744:VAL:HG11	1:C:770:ILE:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:PRO:CD	1:F:462:VAL:HG22	2.30	0.59
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:E:748:GLN:HG3	1:E:769:THR:HB	1.84	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:B:111:ARG:HD2	3:B:1450:HOH:O	2.02	0.58
1:C:332:ILE:CD1	1:C:408:MSE:HE2	2.32	0.58
1:C:745:ASN:C	1:C:745:ASN:HD22	2.11	0.58
1:E:609:MSE:HE1	1:E:615:MSE:CA	2.33	0.58
1:F:79:GLY:CA	1:F:432:ASP:H	2.15	0.58
1:A:169:PHE:O	1:D:225:VAL:HG11	2.04	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:D:749:ASP:O	1:D:764:GLN:HG3	2.03	0.58
1:B:674:ASN:HB3	1:B:680:TYR:CE1	2.37	0.58
1:C:283:GLU:O	1:C:287:ASN:HB2	2.03	0.58
1:F:350:ILE:HD11	1:F:354:SER:HB3	1.85	0.58
1:A:718:ARG:HB2	1:A:723:ILE:HG12	1.85	0.58
1:B:41:VAL:HG12	1:B:41:VAL:O	2.03	0.58
1:D:20:LEU:HD13	1:D:38:PRO:C	2.28	0.58
1:F:497:GLY:O	1:F:500:ILE:HG22	2.03	0.58
1:B:517:ASN:O	1:B:518:THR:HG23	2.04	0.58
1:E:72:PHE:HB2	1:E:235:GLU:CG	2.33	0.58
1:C:589:ARG:NH2	1:C:612:ASP:OD2	2.33	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:A:419:GLU:OE2	1:A:466:ARG:HD2	2.04	0.57
1:B:750:GLY:N	1:B:764:GLN:HG2	2.19	0.57
1:C:495:ARG:NH2	1:F:225:VAL:CG1	2.66	0.57
1:A:293:MSE:HE2	1:A:549:TRP:CH2	2.39	0.57
1:A:332:ILE:HD12	1:A:408:MSE:CE	2.31	0.57
1:A:732:LYS:HD2	1:A:732:LYS:N	2.19	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:D:358:LYS:O	1:D:362:GLU:HG3	2.05	0.57
1:E:244:GLY:HA2	1:E:253:ARG:HH12	1.69	0.57
1:F:732:LYS:CE	1:F:733:ASN:H	2.16	0.57
1:A:43:GLU:HG2	1:A:46:TRP:HB2	1.86	0.57
1:A:601:CYS:HA	1:A:604:LEU:CD2	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:PRO:O	1:B:646:GLY:HA3	2.05	0.57
1:C:265:PRO:CD	1:C:462:VAL:HG22	2.34	0.57
1:D:752:GLN:HG3	1:D:759:LEU:HD11	1.86	0.57
1:D:763:PRO:HB3	1:D:768:LEU:HD11	1.86	0.57
1:D:300:LEU:HD12	1:D:340:LEU:HD22	1.86	0.57
1:E:613:ASN:HD22	1:E:664:ARG:HD3	1.69	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: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:A:474:LYS:O	1:A:476:PRO:HD3	2.05	0.57
1:E:265:PRO:HD2	1:E:462:VAL:HG22	1.85	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:A:123:LEU:N	1:A:123:LEU:HD22	2.19	0.57
1:B:244:GLY:O	1:B:245:PRO:C	2.46	0.57
1:C:495:ARG:HH21	1:F:225:VAL:CG1	2.18	0.57
1:C:535:SER:HA	1:C:587:MSE:HE3	1.86	0.57
1:E:123:LEU:N	1:E:123:LEU:HD22	2.20	0.57
1:E:324:THR:O	1:E:326:PRO:HD3	2.05	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: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:A:494:LEU:HD12	1:A:588:MSE:HE3	1.87	0.56
1:B:265:PRO:HG3	1:B:459:GLU:O	2.05	0.56
1:C:48:LEU:HD12	1:C:49:ASP:HB2	1.86	0.56
1:C:748:GLN:HB3	1:C:769:THR:CG2	2.35	0.56
1:E:367:LEU:HD22	1:E:425:VAL:HG22	1.86	0.56
1:E:747:LEU:HD23	1:E:748:GLN:N	2.21	0.56
1:F:768:LEU:HD12	1:F:769:THR:H	1.69	0.56
1:B:554:GLU:O	1:B:558:VAL:HG23	2.06	0.56
1:D:28:GLN:HG3	1:D:56:ARG:HH12	1.69	0.56
1:B:301:HIS:HE2	1:B:677:ARG:HA	1.70	0.56
1:D:651:LYS:HD3	1:D:651:LYS:C	2.30	0.56
1:F:348:PRO:HD3	1:F:444:TYR:CZ	2.41	0.56
1:F:531:GLY:O	1:F:537:SER:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:273:LEU:HD13	1:F:273:LEU:C	2.31	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:A:46:TRP:HE3	1:A:46:TRP:HA	1.71	0.56
1:A:265:PRO:CD	1:A:462:VAL:HG22	2.36	0.56
1:A:689:HIS:HD2	1:A:739:ARG:HD3	1.71	0.56
1:B:195:LYS:HE2	1:B:478:HIS:HB3	1.87	0.56
1:D:690:LEU:HD11	1:D:693:LEU:CB	2.33	0.56
1:E:287:ASN:O	1:E:290:ILE:HG12	2.06	0.56
1:E:368:LYS:O	1:E:425:VAL:CG2	2.54	0.56
1:D:329:GLU:N	1:D:408:MSE:HE3	2.22	0.55
1:D:282:ASP:OD1	1:D:285:THR:HG23	2.06	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: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:F:244:GLY:O	1:F:245:PRO:C	2.49	0.55
1:A:367:LEU:HD22	1:A:425:VAL:HG22	1.89	0.55
1:B:352:GLN:HA	1:B:357:PHE:CD1	2.42	0.55
1:C:526:ARG:HD2	1:C:619:VAL:HG22	1.89	0.55
1:E:381:GLN:HB2	1:E:384:LEU:HD12	1.88	0.55
1:A:367:LEU:HD22	1:A:425:VAL:CG2	2.37	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:41:VAL:HG21	1:C:313:PHE:HZ	1.72	0.55
1:A:146:GLN:HE21	1:A:146:GLN:HA	1.71	0.55
1:A:592:MSE:HE3	1:A:593:MSE:CA	2.37	0.55
1:A:698:GLU:OE2	1:A:715:LYS:HE2	2.06	0.55
1:B:748:GLN:O	1:B:749:ASP:C	2.50	0.55
1:D:133:GLN:O	1:D:136:ASN:HB2	2.06	0.55
1:D:485:ALA:HB1	1:D:519:ALA:N	2.21	0.55
1:C:703:VAL:HG12	1:C:712:PHE:HB3	1.87	0.55
1:E:745:ASN:C	1:E:745:ASN:HD22	2.15	0.55
1:B:244:GLY:O	1:B:246:THR:N	2.40	0.55
1:D:347:ASN:C	1:D:347:ASN:ND2	2.64	0.55
1:E:200:TYR:CE2	1:E:228:VAL:HG11	2.42	0.55
1:E:342:ILE:HD13	1:E:342:ILE:N	2.20	0.55
1:A:46:TRP:HA	1:A:46:TRP:CE3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:NZ	1:A:478:HIS:HB3	2.21	0.55
1:C:591:MSE:CE	1:C:607:GLN:HE21	2.16	0.55
1:D:165:LEU:HD13	1:D:200:TYR:HB3	1.88	0.55
1:D:273:LEU:HD11	1:D:289:PHE:HE2	1.71	0.55
1:E:134:VAL:O	1:E:135:LYS:HB2	2.06	0.55
1:E:265:PRO:CD	1:E:462:VAL:HG22	2.37	0.55
1:A:244:GLY:C	1:A:246:THR:N	2.65	0.54
1:A:246:THR:HG23	3:A:1042:HOH:O	2.07	0.54
1:B:136:ASN:HB3	1:B:153:ARG:HB2	1.90	0.54
1:B:248:LYS:HG3	1:B:593:MSE:HE3	1.89	0.54
1:B:328:PRO:HB3	1:B:408:MSE:HE1	1.89	0.54
1:E:342:ILE:HD13	1:E:411:ASP:OD1	2.07	0.54
1:F:405:LEU:C	1:F:410:VAL:HG22	2.33	0.54
1:A:170:THR:CG2	1:A:177:GLN:OE1	2.56	0.54
1:A:308:PHE:CD1	1:A:308:PHE:C	2.86	0.54
1:C:67:VAL:O	1:C:238:GLU:HA	2.07	0.54
1:E:733:ASN:N	1:E:733:ASN:ND2	2.49	0.54
1:A:745:ASN:C	1:A:745:ASN:HD22	2.14	0.54
1:A:18:HIS:O	1:A:38:PRO:HA	2.08	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:B:591:MSE:HG2	1:B:604:LEU:HD23	1.90	0.54
1:D:168:ARG:HB2	1:D:174:ARG:NH1	2.23	0.54
1:E:39:ARG:HH22	1:E:46:TRP:HB3	1.72	0.54
1:E:286:VAL:CG2	1:E:331:MSE:HE2	2.36	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:591:MSE:HE1	1:D:608:TYR:CA	2.37	0.54
1:D:745:ASN:C	1:D:745:ASN:HD22	2.14	0.54
1:E:464:PHE:CE2	1:E:538:ARG:HD2	2.43	0.54
1:A:617:ALA:HB3	1:A:660:PRO:HB2	1.89	0.54
1:D:742:VAL:HG23	1:D:743:LYS:H	1.73	0.54
1:F:379:LYS:HE2	1:F:379:LYS:HA	1.90	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:D:390:THR:CG2	1:D:428:PHE:HB3	2.37	0.54
1:D:447:LEU:HD13	1:D:447:LEU:C	2.32	0.54
1:E:152:GLU:HB3	1:E:230:PHE:CE1	2.43	0.54
1:E:320:TRP:O	1:E:322:PRO:HD3	2.08	0.54
1:F:306:ASP:O	1:F:309:TRP:HD1	1.91	0.54
1:A:495:ARG:NH2	1:D:225:VAL:CG1	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:GLN:O	1:A:768:LEU:HB2	2.07	0.54
1:B:50:THR:O	1:F:382:PRO:HG3	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: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
1:F:367:LEU:HG	1:F:425:VAL:HG11	1.89	0.53
1:C:511:ASP:OD1	1:C:538:ARG:HD2	2.08	0.53
1:D:61:GLN:HB2	1:D:64:ILE:HD12	1.90	0.53
1:E:38:PRO:HG3	1:E:51:PRO:HD2	1.90	0.53
1:E:490:MSE:HE2	1:E:620:PHE:CE2	2.43	0.53
1:F:291:ASP:O	1:F:295:GLU:HG3	2.09	0.53
1:F:575:ARG:HG3	1:F:702:GLU:O	2.09	0.53
1:A:279:THR:HG22	1:A:279:THR:O	2.08	0.53
1:C:456:VAL:HG12	1:C:460:GLU:HB2	1.91	0.53
1:A:327:ASP:OD2	1:A:330:GLY:HA3	2.07	0.53
1:C:41:VAL:O	1:C:41:VAL:HG13	2.07	0.53
1:C:88:GLN:CD	1:C:88:GLN:N	2.66	0.53
1:D:684:GLU:CD	1:D:732:LYS:HD2	2.34	0.53
1:D:723:ILE:HB	1:D:770:ILE:HB	1.90	0.53
1:E:273:LEU:HD21	1:E:289:PHE:CE1	2.44	0.53
1:E:752:GLN:HB2	1:E:759:LEU:HD11	1.89	0.53
1:E:768:LEU:HD23	1:E:769:THR:N	2.24	0.53
1:F:389:PHE:HB2	1:F:443:ILE:HD13	1.90	0.53
1:A:222:SER:O	1:D:191:GLU:HG2	2.08	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:B:473:GLN:HG2	1:B:504:GLY:O	2.09	0.53
1:D:265:PRO:HD2	1:D:462:VAL:HG22	1.90	0.53
1:F:601:CYS:HA	1:F:604:LEU:HD22	1.90	0.53
1:F:694:GLN:HB2	1:F:697:HIS:CD2	2.44	0.53
1:D:715:LYS:HB3	1:D:726:THR:HG22	1.89	0.53
1:C:273:LEU:HD13	1:C:273:LEU:C	2.32	0.53
1:C:282:ASP:H	1:C:285:THR:HG22	1.72	0.53
1:E:390:THR:HG21	1:E:427:TRP:HB3	1.89	0.53
1:E:390:THR:HG22	1:E:428:PHE:HB3	1.91	0.53
1:F:723:ILE:HB	1:F:770:ILE:HG13	1.90	0.53
1:A:668:LEU:HB3	1:A:701:CYS:HB2	1.91	0.53
1:F:31:GLU:OE2	1:F:56:ARG:HD3	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HD22	1:A:134:VAL:HG22	1.90	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:D:497:GLY:O	1:D:500:ILE:HG22	2.09	0.53
1:D:566:LYS:HG2	1:D:570:MSE:HE3	1.91	0.53
1:B:719:THR:O	1:B:722:THR:HG22	2.09	0.52
1:C:743:LYS:HA	1:C:759:LEU:CD1	2.38	0.52
1:D:617:ALA:O	1:D:660:PRO:HD2	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:E:201:MSE:HE2	1:E:502:LEU:O	2.08	0.52
1:D:332:ILE:O	1:D:336:LYS:HG3	2.10	0.52
1:A:306:ASP:OD2	1:A:306:ASP:C	2.52	0.52
1:B:714:LEU:HD21	1:B:725:VAL:CG1	2.40	0.52
1:D:591:MSE:HE1	1:D:607:GLN:C	2.34	0.52
1:F:187:GLY:HA2	1:F:482:ASP:OD2	2.09	0.52
1:B:273:LEU:C	1:B:273:LEU:HD13	2.33	0.52
1:C:768:LEU:C	1:C:768:LEU:HD22	2.35	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:B:290:ILE:HD13	1:B:290:ILE:C	2.35	0.52
1:E:730:GLU:HG3	1:E:730:GLU:O	2.09	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:447:LEU:C	1:E:447:LEU:HD13	2.35	0.52
1:C:352:GLN:HA	1:C:357:PHE:CD1	2.45	0.52
1:D:283:GLU:HA	1:D:331:MSE:CE	2.40	0.52
1:E:359:GLU:O	1:E:363:LYS:HG2	2.08	0.52
1:E:594:GLU:HG3	1:E:609:MSE:HG3	1.90	0.52
1:E:595:PHE:CE1	1:E:631:PRO:HG2	2.45	0.52
1:A:150:MSE:CG	1:A:237:LEU:HB2	2.40	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:D:160:GLU:HG3	1:D:204:ARG:HG2	1.92	0.52
1:D:348:PRO:HD3	1:D:444:TYR:CZ	2.45	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:133:GLN:HB2	1:B:136:ASN:HD22	1.75	0.51
1:B:589:ARG:NH2	1:B:612:ASP:OD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:ASN:ND2	1:B:684:GLU:O	2.43	0.51
1:B:689:HIS:HD2	1:B:739:ARG:HD3	1.75	0.51
1:C:377:TRP:CE2	1:C:379:LYS:HB2	2.44	0.51
1:F:343:CYS:HB2	1:F:412:CYS:SG	2.50	0.51
1:C:190:THR:HA	1:F:223:GLU:O	2.10	0.51
1:C:225:VAL:CG1	1:F:495:ARG:NH2	2.74	0.51
1:C:390:THR:CG2	1:C:428:PHE:HB3	2.41	0.51
1:E:502:LEU:HD11	1:E:592:MSE:CE	2.37	0.51
1:C:50:THR:O	1:E:382:PRO:HG3	2.10	0.51
1:E:243:ASP:CG	1:E:244:GLY:N	2.68	0.51
1:A:560:ARG:O	1:A:564:GLN:HG3	2.09	0.51
1:B:267:TRP:CE3	1:B:341:LYS:HG3	2.45	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
1:D:201:MSE:CE	1:D:502:LEU:O	2.59	0.51
1:D:569:MSE:HB3	1:D:573:LEU:HD22	1.91	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:F:759:LEU:C	1:F:759:LEU:HD23	2.35	0.51
1:A:70:GLU:OE2	1:A:73:GLN:NE2	2.31	0.51
1:B:170:THR:HG22	1:E:225:VAL:HG12	1.92	0.51
1:B:225:VAL:HG11	1:E:492:GLU:HG2	1.92	0.51
1:C:48:LEU:HD12	1:C:48:LEU:C	2.36	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:382:PRO:HG3	1:E:50:THR:O	2.11	0.51
1:B:299:PRO:HG2	1:B:676:GLN:OE1	2.11	0.51
1:E:401:LYS:O	1:E:405:LEU:HD13	2.11	0.51
1:F:71:HIS:HD2	1:F:235:GLU:OE1	1.94	0.51
1:F:617:ALA:HB3	1:F:660:PRO:HB2	1.92	0.51
1:B:522:HIS:CE1	1:B:523:VAL:HG23	2.46	0.51
1:B:526:ARG:HD2	1:B:619:VAL:CG2	2.33	0.51
1:E:645:ASP:HB2	1:E:648:ARG:NH2	2.25	0.51
1:F:195:LYS:HB3	1:F:468:ALA:HB3	1.91	0.51
1:A:526:ARG:HD2	1:A:619:VAL:HB	1.93	0.51
1:B:724:THR:HG22	1:B:726:THR:HG23	1.93	0.51
1:C:269:PHE:HE2	1:C:587:MSE:CE	2.21	0.51
1:C:497:GLY:O	1:C:500:ILE:HG22	2.11	0.51
1:E:133:GLN:HB2	1:E:136:ASN:HD22	1.75	0.51
1:E:201:MSE:CE	1:E:502:LEU:O	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:512:ILE:HG12	1:E:538:ARG:O	2.10	0.51
1:C:194:TYR:CD2	1:C:466:ARG:HD3	2.46	0.51
1:D:384:LEU:C	1:D:384:LEU:HD23	2.36	0.51
1:E:44:ARG:HG3	1:E:44:ARG:HH11	1.75	0.51
1:F:332:ILE:HD12	1:F:408:MSE:CE	2.36	0.51
1:C:262:ALA:HB3	1:C:476:PRO:CG	2.39	0.50
1:D:20:LEU:HD13	1:D:38:PRO:O	2.11	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:C:436:MSE:CE	1:C:440:TYR:HA	2.41	0.50
1:B:291:ASP:O	1:B:295:GLU:HG3	2.11	0.50
1:D:273:LEU:HD13	1:D:273:LEU:C	2.37	0.50
1:D:347:ASN:HA	1:D:444:TYR:OH	2.11	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:F:736:LEU:HD13	1:F:736:LEU:C	2.36	0.50
1:E:390:THR:HG23	1:E:429:ASP:H	1.76	0.50
1:B:651:LYS:C	1:B:651:LYS:HD3	2.36	0.50
1:A:449:TRP:CH2	1:A:476:PRO:HD2	2.47	0.50
1:A:754:GLU:HG2	1:A:759:LEU:CD2	2.42	0.50
1:B:738:LEU:N	1:B:738:LEU:HD22	2.27	0.50
1:C:748:GLN:HB3	1:C:769:THR:HG23	1.94	0.50
1:D:18:HIS:O	1:D:38:PRO:HA	2.11	0.50
1:F:282:ASP:O	1:F:286:VAL:HG23	2.11	0.50
1:B:296:ARG:O	1:B:560:ARG:NH1	2.45	0.50
1:C:343:CYS:HB2	1:C:412:CYS:SG	2.51	0.50
1:C:664:ARG:O	1:C:667:THR:CG2	2.59	0.50
1:F:281:TYR:O	1:F:324:THR:HG23	2.11	0.50
1:F:695:ASP:OD1	1:F:720:GLY:N	2.45	0.50
1:A:73:GLN:HG3	1:C:352:GLN:NE2	2.26	0.50
1:A:736:LEU:HD13	1:A:736:LEU:C	2.37	0.50
1:C:485:ALA:CB	1:C:519:ALA:HB2	2.40	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:CB	2.41	0.50
1:E:61:GLN:NE2	1:E:87:LEU:CD2	2.75	0.50
1:E:456:VAL:HG12	1:E:460:GLU:HB2	1.94	0.50
1:A:44:ARG:HH21	1:C:278:THR:CA	2.22	0.49
1:A:768:LEU:C	1:A:768:LEU:HD22	2.37	0.49
1:C:283:GLU:CD	1:C:326:PRO:HD2	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:ARG:O	1:A:718:ARG:HG3	2.10	0.49
1:A:768:LEU:HD13	1:A:768:LEU:N	2.25	0.49
1:B:277:PHE:O	1:B:278:THR:CB	2.57	0.49
1:B:379:LYS:HE2	1:B:379:LYS:CA	2.31	0.49
1:C:416:ASP:O	1:C:416:ASP:OD2	2.30	0.49
1:C:766:ASN:C	1:C:766:ASN:ND2	2.70	0.49
1:E:416:ASP:OD1	1:E:466:ARG:HD3	2.12	0.49
1:E:439:HIS:HD2	3:E:1490:HOH:O	1.94	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
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: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: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: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: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:D:195:LYS:CE	1:D:478:HIS:HB3	2.43	0.49
1:E:738:LEU:HD22	1:E:738:LEU:N	2.28	0.49
1:F:747:LEU:HD22	1:F:770:ILE:CG2	2.42	0.49
1:C:568:ARG:HG2	1:C:568:ARG:HH11	1.77	0.49
1:D:617:ALA:HB3	1:D:660:PRO:HB2	1.95	0.49
1:E:265:PRO:HG3	1:E:460:GLU:HA	1.95	0.49
1:C:332:ILE:O	1:C:336:LYS:HG3	2.13	0.49
1:D:262:ALA:HB3	1:D:476:PRO:CG	2.39	0.49
1:B:31:GLU:HG2	1:B:58:PHE:CB	2.37	0.49
1:B:100:TYR:CG	1:B:111:ARG:HD3	2.48	0.49
1:B:689:HIS:CD2	1:B:739:ARG:NH1	2.79	0.49
1:C:137:ASN:HB3	1:C:152:GLU:OE1	2.13	0.49
1:D:571:PRO:HG2	1:D:672:GLY:N	2.28	0.49
1:A:368:LYS:O	1:A:425:VAL:HG22	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: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:A:134:VAL:O	1:A:135:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:THR:HG23	1:C:303:PHE:HZ	1.77	0.48
1:C:474:LYS:O	1:C:476:PRO:HD3	2.12	0.48
1:D:635:TRP:HB3	1:D:662:TYR:HB3	1.94	0.48
1:A:516:GLU:HB3	1:A:543:LYS:HZ2	1.77	0.48
1:B:694:GLN:HB2	1:B:697:HIS:CD2	2.48	0.48
1:D:368:LYS:O	1:D:425:VAL:CG2	2.61	0.48
1:A:225:VAL:CG1	1:D:495:ARG:NH2	2.76	0.48
1:A:332:ILE:O	1:A:336:LYS:HG3	2.13	0.48
1:A:517:ASN:CG	1:A:518:THR:H	2.22	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:65:VAL:HG21	1:E:108:LEU:HD22	1.96	0.48
1:E:262:ALA:HB3	1:E:476:PRO:HG2	1.93	0.48
1:B:295:GLU:OE2	1:B:296:ARG:HG3	2.13	0.48
1:C:163:TYR:HB3	1:C:502:LEU:HD13	1.95	0.48
1:C:276:SER:HB2	1:C:279:THR:OG1	2.12	0.48
1:C:635:TRP:O	1:C:643:GLU:HA	2.14	0.48
1:A:41:VAL:HG22	1:A:47:GLN:CG	2.43	0.48
1:B:416:ASP:OD2	1:B:466:ARG:HD3	2.13	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:D:744:VAL:HG22	1:D:759:LEU:CD2	2.43	0.48
1:E:44:ARG:HA	1:E:47:GLN:CG	2.44	0.48
1:E:261:PRO:HA	1:E:473:GLN:O	2.12	0.48
1:E:279:THR:O	1:E:279:THR:HG22	2.13	0.48
1:F:16:LEU:HD22	1:F:140:VAL:HG22	1.94	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:B:488:GLU:O	1:B:492:GLU:HG3	2.14	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:A:401:LYS:HB2	1:A:401:LYS:HZ2	1.79	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: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:D:570:MSE:HE1	1:D:573:LEU:HD23	1.92	0.48
1:E:355:PRO:O	1:E:358:LYS:HE2	2.13	0.48
1:F:687:ALA:HA	1:F:735:THR:HG23	1.96	0.48
1:B:141:GLN:HA	1:B:148:ASN:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:HIS:HA	3:C:1154:HOH:O	2.13	0.48
1:E:388:ASP:C	1:E:390:THR:H	2.21	0.48
1:F:405:LEU:O	1:F:410:VAL:HG22	2.13	0.48
1:B:651:LYS:HD3	1:B:652:GLN:N	2.29	0.48
1:C:265:PRO:HG3	1:C:459:GLU:O	2.13	0.48
1:E:474:LYS:O	1:E:476:PRO:HD3	2.12	0.48
1:F:425:VAL:CG1	1:F:426:GLN:H	2.26	0.48
1:B:156:LEU:HD11	1:B:228:VAL:HG23	1.95	0.47
1:B:298:LEU:N	1:B:299:PRO:HD3	2.28	0.47
1:B:755:SER:O	1:B:756:GLU:C	2.57	0.47
1:C:517:ASN:HD22	1:C:517:ASN:HA	1.53	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: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:A:262:ALA:HB3	1:A:476:PRO:CG	2.42	0.47
1:A:321:ASP:HB3	1:A:324:THR:OG1	2.13	0.47
1:D:200:TYR:CE2	1:D:228:VAL:HG11	2.49	0.47
1:E:290:ILE:HD11	1:E:338:LYS:NZ	2.28	0.47
1:E:336:LYS:O	1:E:337:ALA:C	2.54	0.47
1:E:733:ASN:HD22	1:E:733:ASN:H	1.59	0.47
1:F:406:VAL:HA	1:F:410:VAL:HG22	1.95	0.47
1:D:273:LEU:HD13	1:D:274:THR:N	2.29	0.47
1:E:78:ASN:O	1:E:435:LYS:HE3	2.14	0.47
1:F:262:ALA:HB3	1:F:476:PRO:CG	2.43	0.47
1:A:447:LEU:HD13	1:A:447:LEU:C	2.39	0.47
1:A:745:ASN:C	1:A:745:ASN:ND2	2.72	0.47
1:B:29:ASP:CG	1:B:30:ASN:N	2.71	0.47
1:B:384:LEU:C	1:B:384:LEU:HD23	2.40	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:E:526:ARG:CZ	1:E:619:VAL:HG21	2.45	0.47
1:A:280:ASN:HB2	1:A:308:PHE:CE2	2.50	0.47
1:A:502:LEU:CD1	1:A:592:MSE:HE2	2.29	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:D:377:TRP:CE2	1:D:379:LYS:HB2	2.49	0.47
1:E:720:GLY:C	1:E:721:ASN:HD22	2.22	0.47
1:A:279:THR:CG2	1:A:546:ARG:NH1	2.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LYS:NZ	1:A:453:LYS:HB3	2.29	0.47
1:B:123:LEU:HD23	1:B:128:ARG:HA	1.96	0.47
1:B:730:GLU:HG2	1:B:732:LYS:HE2	1.96	0.47
1:D:335:LEU:O	1:D:338:LYS:HB2	2.14	0.47
1:D:591:MSE:HE1	1:D:608:TYR:HA	1.95	0.47
1:E:41:VAL:HG22	1:E:41:VAL:O	2.14	0.47
1:E:101:ALA:HB3	1:E:112:VAL:CG1	2.45	0.47
1:E:244:GLY:O	1:E:245:PRO:C	2.57	0.47
1:F:275:THR:HG21	1:F:280:ASN:OD1	2.13	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:156:LEU:CD1	1:B:228:VAL:HG23	2.44	0.47
1:B:262:ALA:HB3	1:B:476:PRO:CG	2.43	0.47
1:C:283:GLU:HA	1:C:331:MSE:HE1	1.96	0.47
1:C:292:GLY:O	1:C:296:ARG:NH1	2.46	0.47
1:C:487:TYR:OH	1:C:522:HIS:HD2	1.98	0.47
1:C:500:ILE:HG12	1:C:505:PHE:HB2	1.97	0.47
1:D:273:LEU:HD23	1:D:539:LEU:HB3	1.96	0.47
1:F:377:TRP:CE2	1:F:379:LYS:HB2	2.50	0.47
1:A:41:VAL:O	1:A:41:VAL:HG13	2.14	0.47
1:B:439:HIS:HD2	3:B:1268:HOH:O	1.98	0.47
1:C:29:ASP:O	1:C:30:ASN:HB2	2.15	0.47
1:C:279:THR:HA	1:C:281:TYR:CZ	2.50	0.47
1:D:668:LEU:HD13	1:D:690:LEU:HD23	1.97	0.47
1:E:80:PRO:HD3	1:E:431:SER:HB3	1.96	0.47
1:F:237:LEU:HD13	1:F:237:LEU:C	2.40	0.47
1:F:694:GLN:O	1:F:697:HIS:HB2	2.13	0.47
1:F:745:ASN:H	1:F:745:ASN:HD22	1.63	0.47
1:A:222:SER:O	1:D:191:GLU:CG	2.62	0.47
1:A:279:THR:O	1:A:279:THR:CG2	2.63	0.47
1:A:310:MSE:HE1	1:A:316:CYS:CA	2.44	0.47
1:B:133:GLN:HB2	1:B:136:ASN:ND2	2.30	0.47
1:C:290:ILE:CD1	1:C:338:LYS:HD2	2.45	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:A:500:ILE:HG12	1:A:505:PHE:HB2	1.98	0.46
1:B:296:ARG:O	1:B:298:LEU:HG	2.14	0.46
1:D:419:GLU:HG3	1:D:467:SER:OG	2.15	0.46
1:F:345:TRP:CH2	1:F:347:ASN:ND2	2.83	0.46
1:C:183:ASN:HA	1:C:196:ASN:ND2	2.30	0.46
1:C:225:VAL:HG11	1:F:169:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:LYS:HB2	1:D:396:LYS:NZ	2.30	0.46
1:D:436:MSE:HE1	1:D:443:ILE:HD12	1.96	0.46
1:E:277:PHE:C	1:E:278:THR:HG23	2.40	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: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:B:591:MSE:HE1	1:B:607:GLN:C	2.40	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:F:165:LEU:HA	1:F:197:ILE:O	2.16	0.46
1:A:244:GLY:O	1:A:246:THR:N	2.49	0.46
1:A:735:THR:HG22	1:A:762:LYS:HG2	1.98	0.46
1:B:569:MSE:HB2	1:B:573:LEU:HD22	1.97	0.46
1:B:766:ASN:O	1:B:767:ALA:HB2	2.16	0.46
1:C:153:ARG:HG2	1:C:229:GLN:HB2	1.96	0.46
1:C:384:LEU:C	1:C:384:LEU:HD23	2.41	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:A:15:ASN:HB2	1:A:141:GLN:HE21	1.79	0.46
1:A:308:PHE:C	1:A:308:PHE:HD1	2.23	0.46
1:A:635:TRP:HB3	1:A:662:TYR:HB3	1.98	0.46
1:C:752:GLN:HB2	1:C:759:LEU:HD21	1.98	0.46
1:E:292:GLY:O	1:E:296:ARG:HD3	2.16	0.46
1:F:137:ASN:HB3	1:F:152:GLU:CD	2.41	0.46
1:F:252:ASP:HA	1:F:583:ARG:O	2.14	0.46
1:F:526:ARG:CD	1:F:619:VAL:HG22	2.36	0.46
1:A:367:LEU:HD21	1:A:425:VAL:HG13	1.96	0.46
1:A:747:LEU:HD21	1:A:750:GLY:O	2.14	0.46
1:B:273:LEU:HD23	1:B:539:LEU:HB3	1.96	0.46
1:C:225:VAL:HG13	1:F:495:ARG:NH2	2.30	0.46
1:C:273:LEU:HD13	1:C:274:THR:N	2.31	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:B:80:PRO:HD3	1:B:431:SER:HB3	1.98	0.46
1:B:248:LYS:CG	1:B:593:MSE:HE3	2.46	0.46
1:B:591:MSE:HE1	1:B:608:TYR:HA	1.98	0.46
1:C:314:GLN:HB3	1:C:354:SER:HB2	1.97	0.46
1:C:331:MSE:HA	1:C:334:ARG:HH11	1.79	0.46
1:D:163:TYR:HB3	1:D:502:LEU:HD13	1.96	0.46
1:E:502:LEU:HD13	1:E:593:MSE:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:419:GLU:OE2	1:F:466:ARG:HD2	2.16	0.46
1:B:223:GLU:O	1:E:190:THR:HA	2.16	0.46
1:B:278:THR:HG23	1:D:44:ARG:CD	2.45	0.46
1:B:664:ARG:HG3	1:B:665:ASP:N	2.30	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:E:646:GLY:O	1:E:647:SER:HB2	2.16	0.46
1:A:734:TRP:CZ2	1:A:763:PRO:HG3	2.51	0.46
1:B:332:ILE:HG23	1:B:342:ILE:HG13	1.97	0.46
1:C:76:LEU:CD2	1:E:373:SER:HB3	2.33	0.46
1:C:296:ARG:HG3	1:C:296:ARG:HH11	1.79	0.46
1:C:402:LEU:HB3	1:C:451:VAL:HG11	1.98	0.46
1:D:41:VAL:HG22	1:D:47:GLN:HG2	1.98	0.46
1:D:512:ILE:HG21	1:D:528:CYS:SG	2.55	0.46
1:F:277:PHE:O	1:F:278:THR:OG1	2.30	0.46
1:F:512:ILE:HD12	1:F:512:ILE:N	2.31	0.46
1:A:319:GLU:OE2	1:A:356:VAL:HG23	2.15	0.46
1:C:296:ARG:O	1:C:298:LEU:HD13	2.16	0.46
1:E:635:TRP:CH2	1:E:664:ARG:HB3	2.51	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:65:VAL:CG2	1:E:108:LEU:HD22	2.46	0.45
1:E:137:ASN:HB3	1:E:152:GLU:OE2	2.16	0.45
1:E:160:GLU:HG3	1:E:204:ARG:HG2	1.98	0.45
1:E:183:ASN:HA	1:E:196:ASN:ND2	2.31	0.45
1:E:310:MSE:SE	1:E:316:CYS:H	2.48	0.45
1:C:463:LEU:O	1:C:477:VAL:HB	2.15	0.45
1:C:734:TRP:CH2	1:C:763:PRO:HG2	2.51	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:D:494:LEU:HD22	1:D:498:LEU:HG	1.98	0.45
1:E:295:GLU:C	1:E:297:ASN:N	2.74	0.45
1:E:397:TRP:CZ2	1:E:401:LYS:HE2	2.52	0.45
1:B:243:ASP:CG	1:B:244:GLY:H	2.25	0.45
1:B:490:MSE:HE2	1:B:620:PHE:CE2	2.50	0.45
1:B:638:LEU:HD12	1:B:639:TRP:CE3	2.50	0.45
1:D:732:LYS:O	1:D:733:ASN:HB2	2.16	0.45
1:E:278:THR:HG22	1:E:308:PHE:CD2	2.50	0.45
1:F:367:LEU:HD11	1:F:425:VAL:CG1	2.44	0.45
1:F:745:ASN:HD22	1:F:745:ASN:C	2.24	0.45
1:A:191:GLU:HB3	1:D:222:SER:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:LEU:HD11	1:B:608:TYR:HB3	1.98	0.45
1:B:630:LEU:O	1:B:647:SER:N	2.49	0.45
1:D:408:MSE:HE2	1:D:408:MSE:HB3	1.81	0.45
1:E:749:ASP:C	1:E:764:GLN:HG2	2.42	0.45
1:A:273:LEU:HB3	1:A:300:LEU:HD11	1.96	0.45
1:A:306:ASP:CG	1:A:308:PHE:CD2	2.95	0.45
1:B:591:MSE:HE3	1:B:607:GLN:HE21	1.81	0.45
1:C:133:GLN:O	1:C:136:ASN:HB2	2.17	0.45
1:D:753:ALA:O	1:D:759:LEU:HD12	2.17	0.45
1:E:182:TRP:CE3	1:E:215:CYS:HB2	2.52	0.45
1:A:43:GLU:CD	1:A:46:TRP:HD1	2.25	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:275:THR:O	1:A:276:SER:C	2.59	0.45
1:C:449:TRP:CH2	1:C:476:PRO:HD2	2.52	0.45
1:D:718:ARG:HG3	1:D:723:ILE:HD13	1.99	0.45
1:D:725:VAL:HB	1:D:768:LEU:HB2	1.97	0.45
1:F:164:GLY:O	1:F:165:LEU:HB2	2.16	0.45
1:A:436:MSE:HE3	1:A:440:TYR:HB2	1.97	0.45
1:A:670:ALA:HB2	1:A:701:CYS:SG	2.57	0.45
1:B:195:LYS:CE	1:B:478:HIS:HB3	2.46	0.45
1:B:252:ASP:HA	1:B:583:ARG:O	2.16	0.45
1:C:568:ARG:HG2	1:C:568:ARG:NH1	2.32	0.45
1:D:388:ASP:CG	1:D:390:THR:HG22	2.42	0.45
1:E:265:PRO:CG	1:E:460:GLU:HA	2.46	0.45
1:F:61:GLN:HB2	1:F:64:ILE:HD12	1.99	0.45
1:A:306:ASP:OD2	1:A:308:PHE:CD2	2.69	0.45
1:B:127:GLU:OE2	1:B:127:GLU:HA	2.16	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:B:691:PHE:O	1:B:692:ASN:C	2.60	0.45
1:C:348:PRO:HG2	1:C:349:TYR:CE1	2.52	0.45
1:D:134:VAL:HG22	1:D:135:LYS:HG2	1.98	0.45
1:D:390:THR:OG1	1:D:429:ASP:CG	2.60	0.45
1:E:335:LEU:HD13	1:E:335:LEU:HA	1.86	0.45
1:F:490:MSE:HE2	1:F:620:PHE:CD2	2.52	0.45
1:A:497:GLY:C	1:A:588:MSE:HE2	2.41	0.45
1:B:524:TYR:OH	1:B:539:LEU:HD21	2.17	0.45
1:C:653:GLN:HE21	1:C:653:GLN:HB3	1.51	0.45
1:E:335:LEU:O	1:E:338:LYS:HB3	2.17	0.45
1:F:682:TRP:O	1:F:686:THR:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:HZ2	1:A:478:HIS:HB3	1.81	0.44
1:A:276:SER:HA	1:A:541:GLY:O	2.17	0.44
1:B:673:ASN:HD22	1:B:685:GLY:HA3	1.82	0.44
1:B:674:ASN:HB3	1:B:680:TYR:CD1	2.52	0.44
1:E:265:PRO:HD2	1:E:462:VAL:CG2	2.46	0.44
1:E:290:ILE:O	1:E:293:MSE:HB2	2.17	0.44
1:F:78:ASN:HB3	1:F:79:GLY:H	1.41	0.44
1:F:568:ARG:NH1	1:F:672:GLY:O	2.50	0.44
1:F:695:ASP:HA	1:F:718:ARG:HD3	1.99	0.44
1:B:464:PHE:CE2	1:B:477:VAL:HG11	2.52	0.44
1:C:164:GLY:O	1:C:165:LEU:HB2	2.18	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:D:512:ILE:HD12	1:D:531:GLY:HA3	1.99	0.44
1:E:59:SER:HA	1:E:60:PRO:HD3	1.84	0.44
1:C:483:CYS:HB3	1:C:489:SER:OG	2.16	0.44
1:D:749:ASP:C	1:D:764:GLN:HG3	2.42	0.44
1:F:405:LEU:HB3	1:F:410:VAL:HG21	1.99	0.44
1:A:182:TRP:CE3	1:A:215:CYS:HB2	2.53	0.44
1:C:419:GLU:OE2	1:C:466:ARG:HD3	2.17	0.44
1:E:510:HIS:N	1:E:510:HIS:CD2	2.86	0.44
1:E:554:GLU:O	1:E:558:VAL:HG23	2.17	0.44
1:A:18:HIS:HB2	1:A:20:LEU:HD21	1.99	0.44
1:B:328:PRO:HB2	1:B:408:MSE:HE1	1.99	0.44
1:C:502:LEU:HD21	1:C:592:MSE:CE	2.45	0.44
1:C:759:LEU:C	1:C:759:LEU:HD23	2.43	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:A:5:ASP:HB3	1:A:9:LEU:HB2	2.00	0.44
1:A:50:THR:O	1:C:382:PRO:HG3	2.18	0.44
1:A:194:TYR:CE2	1:A:466:ARG:HD3	2.53	0.44
1:B:93:THR:HG23	1:B:104:LYS:HB3	2.00	0.44
1:B:310:MSE:SE	1:B:316:CYS:H	2.51	0.44
1:B:453:LYS:NZ	1:B:458:GLU:HG3	2.32	0.44
1:B:755:SER:O	1:B:757:GLN:N	2.50	0.44
1:C:189:SER:OG	1:F:7:ASN:ND2	2.38	0.44
1:C:436:MSE:HE3	1:C:440:TYR:N	2.32	0.44
1:C:591:MSE:HE3	1:C:607:GLN:HG3	1.99	0.44
1:D:134:VAL:C	1:D:135:LYS:HG2	2.42	0.44
1:F:230:PHE:HE1	1:F:237:LEU:HD11	1.83	0.44
1:F:265:PRO:HG3	1:F:460:GLU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLY:C	1:B:246:THR:N	2.76	0.44
1:C:276:SER:HB2	1:C:279:THR:CG2	2.48	0.44
1:D:80:PRO:HD3	1:D:431:SER:HB3	1.99	0.44
1:E:118:TRP:CD1	1:E:118:TRP:C	2.95	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:C:278:THR:O	1:C:279:THR:HG23	2.17	0.44
1:C:447:LEU:HD13	1:C:447:LEU:C	2.43	0.44
1:D:402:LEU:HB3	1:D:451:VAL:HG11	2.00	0.44
1:E:575:ARG:O	1:E:578:ALA:HB3	2.18	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:A:160:GLU:HA	1:A:203:ASN:OD1	2.18	0.44
1:A:279:THR:HG23	1:A:546:ARG:HH12	1.81	0.44
1:C:309:TRP:HA	1:C:325:PHE:CE1	2.53	0.44
1:C:683:HIS:CD2	1:C:711:ILE:HD13	2.53	0.44
1:D:591:MSE:CE	1:D:608:TYR:HA	2.48	0.44
1:E:674:ASN:HB3	1:E:680:TYR:CE1	2.53	0.44
1:F:747:LEU:HD21	1:F:761:VAL:CG1	2.48	0.44
1:B:648:ARG:HG3	1:B:648:ARG:HH11	1.83	0.43
1:E:539:LEU:HD23	1:E:540:HIS:N	2.33	0.43
1:E:557:ASP:OD1	1:E:560:ARG:NH2	2.51	0.43
1:E:718:ARG:HD3	1:E:720:GLY:O	2.18	0.43
1:F:502:LEU:HD13	1:F:593:MSE:CE	2.48	0.43
1:F:719:THR:O	1:F:719:THR:HG23	2.16	0.43
1:A:488:GLU:CD	1:A:488:GLU:H	2.27	0.43
1:A:598:ASP:HA	1:A:599:PRO:HD3	1.84	0.43
1:D:48:LEU:C	1:D:48:LEU:HD12	2.42	0.43
1:F:200:TYR:CE2	1:F:228:VAL:HG11	2.52	0.43
1:F:747:LEU:HD21	1:F:761:VAL:HG13	2.00	0.43
1:B:137:ASN:HB3	1:B:152:GLU:OE1	2.18	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:E:154:LEU:HD12	1:E:154:LEU:HA	1.84	0.43
1:E:748:GLN:HE21	1:E:748:GLN:HB3	1.60	0.43
1:F:598:ASP:HA	1:F:599:PRO:HD3	1.89	0.43
1:A:594:GLU:C	1:A:596:PRO:HD3	2.43	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:E:16:LEU:CD2	1:E:140:VAL:HG22	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:GLU:OE2	1:E:191:GLU:N	2.44	0.43
1:E:475:PHE:N	1:E:476:PRO:HD3	2.32	0.43
1:F:134:VAL:O	1:F:135:LYS:HB2	2.18	0.43
1:A:137:ASN:HB3	1:A:152:GLU:OE1	2.18	0.43
1:C:723:ILE:HB	1:C:770:ILE:HG23	1.99	0.43
1:C:744:VAL:HG11	1:C:770:ILE:CD1	2.48	0.43
1:D:488:GLU:O	1:D:492:GLU:HG3	2.18	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: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:F:568:ARG:HG2	1:F:568:ARG:HH11	1.84	0.43
1:A:348:PRO:HD3	1:A:444:TYR:CZ	2.53	0.43
1:A:695:ASP:HA	1:A:718:ARG:HG3	2.00	0.43
1:A:754:GLU:HG2	1:A:759:LEU:HD21	2.01	0.43
1:B:18:HIS:O	1:B:38:PRO:HA	2.18	0.43
1:B:354:SER:HA	1:B:355:PRO:HD3	1.92	0.43
1:C:219:GLU:HB2	1:C:229:GLN:HB3	2.00	0.43
1:C:290:ILE:O	1:C:293:MSE:HB2	2.18	0.43
1:C:768:LEU:HD13	1:C:768:LEU:H	1.83	0.43
1:D:104:LYS:HE2	1:D:106:GLY:O	2.19	0.43
1:D:668:LEU:O	1:D:701:CYS:HB2	2.18	0.43
1:D:735:THR:OG1	1:D:760:VAL:HG13	2.19	0.43
1:D:744:VAL:HG22	1:D:759:LEU:HD21	2.00	0.43
1:F:277:PHE:CD2	1:F:278:THR:HG23	2.54	0.43
1:F:743:LYS:HA	1:F:759:LEU:HD12	1.99	0.43
1:A:542:SER:O	1:A:543:LYS:C	2.62	0.43
1:A:673:ASN:N	1:A:673:ASN:HD22	2.14	0.43
1:B:510:HIS:N	1:B:510:HIS:CD2	2.87	0.43
1:F:341:LYS:C	1:F:342:ILE:HD12	2.43	0.43
1:A:136:ASN:HB3	1:A:153:ARG:HB2	2.00	0.43
1:A:498:LEU:O	1:A:502:LEU:HD23	2.19	0.43
1:A:734:TRP:CH2	1:A:763:PRO:HG3	2.53	0.43
1:D:401:LYS:HA	1:D:401:LYS:HD3	1.81	0.43
1:E:244:GLY:CA	1:E:253:ARG:HH12	2.31	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:E:745:ASN:O	1:E:745:ASN:ND2	2.52	0.43
1:A:251:LEU:HD11	1:A:593:MSE:HE2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ASP:OD2	1:B:560:ARG:NH2	2.52	0.43
1:C:282:ASP:H	1:C:285:THR:HG21	1.81	0.43
1:A:165:LEU:HA	1:A:197:ILE:O	2.19	0.43
1:A:320:TRP:O	1:A:322:PRO:HD3	2.19	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:D:246:THR:HG22	1:D:249:ALA:CB	2.49	0.43
1:D:283:GLU:HA	1:D:331:MSE:HE3	2.01	0.43
1:E:335:LEU:C	1:E:336:LYS:O	2.61	0.43
1:E:367:LEU:HD13	1:E:425:VAL:HG21	2.01	0.43
1:E:488:GLU:CD	1:E:488:GLU:H	2.27	0.43
1:A:28:GLN:O	1:A:29:ASP:HB2	2.19	0.42
1:A:377:TRP:HH2	1:A:420:ARG:HD3	1.82	0.42
1:E:498:LEU:O	1:E:502:LEU:HD22	2.19	0.42
1:F:458:GLU:C	1:F:458:GLU:OE2	2.62	0.42
1:F:635:TRP:HB3	1:F:662:TYR:HB3	2.00	0.42
1:A:200:TYR:CE2	1:A:228:VAL:HG11	2.53	0.42
1:A:306:ASP:O	1:A:309:TRP:HD1	2.03	0.42
1:A:348:PRO:HG2	1:A:349:TYR:CE2	2.54	0.42
1:C:641:ASN:OD1	1:C:739:ARG:HD2	2.18	0.42
1:D:152:GLU:HB3	1:D:230:PHE:CE1	2.54	0.42
1:D:745:ASN:H	1:D:745:ASN:ND2	2.17	0.42
1:F:379:LYS:O	1:F:380:TRP:HB3	2.19	0.42
1:A:2:LYS:HD3	1:A:2:LYS:HA	1.74	0.42
1:A:100:TYR:CD1	1:A:100:TYR:C	2.97	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:C:275:THR:HG23	1:C:303:PHE:CZ	2.53	0.42
1:C:390:THR:HG22	1:C:428:PHE:HB3	2.01	0.42
1:C:627:GLN:NE2	1:F:599:PRO:HG3	2.34	0.42
1:D:264:PRO:HG3	1:D:476:PRO:HB3	2.01	0.42
1:D:356:VAL:HG23	1:D:359:GLU:OE2	2.19	0.42
1:E:219:GLU:HB2	1:E:229:GLN:HB3	2.01	0.42
1:F:290:ILE:HD13	1:F:340:LEU:CD1	2.50	0.42
1:F:384:LEU:C	1:F:384:LEU:HD23	2.44	0.42
1:A:139:TYR:CD1	1:A:150:MSE:HE1	2.55	0.42
1:B:2:LYS:HA	1:B:223:GLU:OE2	2.18	0.42
1:B:41:VAL:HG11	1:F:313:PHE:HZ	1.84	0.42
1:B:750:GLY:HA2	1:B:764:GLN:H	1.83	0.42
1:B:763:PRO:C	1:B:765:GLY:H	2.26	0.42
1:C:16:LEU:CD2	1:C:140:VAL:HG22	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:LEU:HD22	1:C:87:LEU:N	2.35	0.42
1:C:617:ALA:HB3	1:C:660:PRO:HB2	2.01	0.42
1:D:378:ASP:OD2	1:F:71:HIS:HE1	2.02	0.42
1:D:479:TRP:CZ3	1:D:481:GLY:HA2	2.54	0.42
1:E:691:PHE:O	1:E:692:ASN:C	2.62	0.42
1:B:641:ASN:ND2	1:B:757:GLN:CG	2.71	0.42
1:C:388:ASP:C	1:C:390:THR:H	2.27	0.42
1:F:627:GLN:HA	1:F:650:HIS:O	2.20	0.42
1:B:76:LEU:HG	1:F:373:SER:HB3	2.02	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:C:591:MSE:HE2	1:C:608:TYR:HA	2.00	0.42
1:C:691:PHE:O	1:C:692:ASN:C	2.62	0.42
1:D:320:TRP:O	1:D:322:PRO:HD3	2.20	0.42
1:A:310:MSE:CE	1:A:318:PHE:H	2.32	0.42
1:A:310:MSE:HE2	1:A:310:MSE:HB3	1.89	0.42
1:A:747:LEU:C	1:A:747:LEU:HD22	2.45	0.42
1:B:275:THR:O	1:B:276:SER:C	2.63	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:F:243:ASP:CG	1:F:244:GLY:N	2.77	0.42
1:F:388:ASP:OD1	1:F:390:THR:OG1	2.34	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:B:64:ILE:CD1	1:B:242:ILE:HD12	2.50	0.42
1:B:273:LEU:HD11	1:B:289:PHE:CE1	2.55	0.42
1:C:592:MSE:SE	1:C:592:MSE:C	3.13	0.42
1:D:685:GLY:HA2	1:D:733:ASN:O	2.20	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:A:342:ILE:HG13	1:A:410:VAL:HA	2.01	0.42
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:B:521:ALA:O	1:B:525:LYS:HG3	2.20	0.42
1:C:123:LEU:HD13	1:C:128:ARG:HA	2.02	0.42
1:C:364:GLY:HA2	3:C:1069:HOH:O	2.19	0.42
1:D:1:MSE:HE1	1:D:149:TYR:CZ	2.55	0.42
1:D:715:LYS:HG2	1:D:716:ALA:N	2.34	0.42
1:A:282:ASP:OD2	1:A:285:THR:HG23	2.20	0.42
1:B:539:LEU:HB3	1:B:540:HIS:H	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:GLU:O	1:C:45:THR:O	2.38	0.42
1:C:225:VAL:HG13	1:F:495:ARG:HH21	1.84	0.42
1:E:41:VAL:CG2	1:E:47:GLN:HA	2.50	0.42
1:E:208:VAL:HA	1:E:240:PHE:O	2.20	0.42
1:A:718:ARG:HD2	1:A:720:GLY:O	2.19	0.41
1:B:416:ASP:OD2	1:B:416:ASP:O	2.38	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: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:E:296:ARG:HB3	1:E:298:LEU:HD23	2.01	0.41
1:E:377:TRP:CE2	1:E:379:LYS:HB2	2.55	0.41
1:F:488:GLU:CD	1:F:488:GLU:H	2.28	0.41
1:A:300:LEU:HD22	1:A:300:LEU:HA	1.90	0.41
1:A:323:LEU:HD22	1:A:323:LEU:N	2.35	0.41
1:A:742:VAL:O	1:A:759:LEU:HD23	2.21	0.41
1:B:271:LEU:C	1:B:271:LEU:HD13	2.45	0.41
1:B:331:MSE:HA	1:B:334:ARG:NH1	2.35	0.41
1:B:768:LEU:HD23	1:B:768:LEU:C	2.44	0.41
1:C:55:LEU:HG	1:C:69:ILE:HG12	2.02	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:E:136:ASN:HB3	1:E:153:ARG:HB2	2.01	0.41
1:F:243:ASP:CG	1:F:244:GLY:H	2.28	0.41
1:F:566:LYS:HA	1:F:569:MSE:CE	2.45	0.41
1:A:20:LEU:O	1:A:118:TRP:HB2	2.21	0.41
1:B:539:LEU:O	1:B:540:HIS:CB	2.68	0.41
1:D:570:MSE:HG3	1:D:678:PRO:HA	2.02	0.41
1:E:539:LEU:HD23	1:E:539:LEU:C	2.44	0.41
1:F:220:VAL:HG13	1:F:228:VAL:HG22	2.00	0.41
1:B:116:GLU:N	1:B:116:GLU:CD	2.79	0.41
1:B:463:LEU:O	1:B:464:PHE:HD2	2.03	0.41
1:C:524:TYR:OH	1:C:539:LEU:HD11	2.20	0.41
1:C:535:SER:CA	1:C:587:MSE:HE3	2.49	0.41
1:D:76:LEU:HD12	1:D:76:LEU:HA	1.82	0.41
1:D:352:GLN:NE2	1:F:73:GLN:HG3	2.35	0.41
1:E:388:ASP:OD1	1:E:390:THR:HB	2.20	0.41
1:F:669:LEU:HD23	1:F:669:LEU:HA	1.92	0.41
1:A:689:HIS:CD2	1:A:739:ARG:HD3	2.52	0.41
1:A:752:GLN:HB2	1:A:759:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:LEU:O	1:C:118:TRP:HB2	2.21	0.41
1:C:272:TRP:HB2	1:C:538:ARG:HA	2.01	0.41
1:C:665:ASP:O	1:C:667:THR:HG22	2.21	0.41
1:D:122:PHE:C	1:D:123:LEU:HD12	2.46	0.41
1:E:358:LYS:O	1:E:362:GLU:HG3	2.21	0.41
1:E:608:TYR:C	1:E:609:MSE:HE2	2.45	0.41
1:F:425:VAL:HG13	1:F:426:GLN:H	1.86	0.41
1:A:306:ASP:OD2	1:A:307:CYS:N	2.54	0.41
1:A:342:ILE:HD11	1:A:410:VAL:HG12	2.03	0.41
1:B:378:ASP:OD1	1:D:71:HIS:HE1	2.04	0.41
1:C:80:PRO:HD3	1:C:431:SER:HB3	2.02	0.41
1:C:610:LEU:HD23	1:C:610:LEU:HA	1.94	0.41
1:C:730:GLU:OE2	1:C:730:GLU:HA	2.19	0.41
1:D:749:ASP:O	1:D:763:PRO:HA	2.21	0.41
1:F:345:TRP:HH2	1:F:347:ASN:ND2	2.18	0.41
1:A:265:PRO:HG3	1:A:459:GLU:O	2.20	0.41
1:A:318:PHE:HB2	1:A:401:LYS:HG2	2.02	0.41
1:A:405:LEU:C	1:A:410:VAL:HG22	2.45	0.41
1:B:475:PHE:N	1:B:476:PRO:HD3	2.34	0.41
1:B:649:TRP:CD1	1:E:600:ALA:HB2	2.55	0.41
1:C:121:ASP:OD1	1:C:128:ARG:HD2	2.20	0.41
1:C:173:VAL:HB	3:C:1086:HOH:O	2.20	0.41
1:C:281:TYR:N	1:C:285:THR:HG21	2.35	0.41
1:D:82:TYR:CE2	1:D:470:VAL:HB	2.55	0.41
1:D:309:TRP:CE2	1:D:310:MSE:HE2	2.55	0.41
1:F:182:TRP:CE3	1:F:215:CYS:HB2	2.55	0.41
1:F:232:VAL:HG12	1:F:237:LEU:HD23	2.03	0.41
1:F:246:THR:HG23	1:F:249:ALA:CB	2.50	0.41
1:F:262:ALA:O	1:F:264:PRO:HD3	2.21	0.41
1:F:358:LYS:HE2	1:F:358:LYS:HB3	1.91	0.41
1:A:275:THR:HG21	1:A:280:ASN:CG	2.43	0.41
1:A:380:TRP:CH2	2:A:801:MES:H21	2.55	0.41
1:A:518:THR:CG2	1:A:519:ALA:H	2.28	0.41
1:A:533:LEU:HD12	1:A:533:LEU:HA	1.85	0.41
1:B:591:MSE:CE	1:B:608:TYR:HA	2.51	0.41
1:C:262:ALA:HB3	1:C:476:PRO:CD	2.51	0.41
1:C:327:ASP:OD2	1:C:330:GLY:HA3	2.20	0.41
1:C:506:GLY:HA2	1:C:586:PRO:HA	2.02	0.41
1:D:275:THR:HA	1:D:541:GLY:HA3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:664:ARG:HG2	1:F:665:ASP:N	2.36	0.41
1:F:723:ILE:HB	1:F:770:ILE:CG1	2.50	0.41
1:A:296:ARG:HD2	1:A:549:TRP:CZ3	2.56	0.41
1:B:41:VAL:HG12	1:B:47:GLN:CG	2.50	0.41
1:B:161:THR:O	1:B:202:THR:HA	2.20	0.41
1:B:273:LEU:HD23	1:B:539:LEU:HD13	2.03	0.41
1:B:764:GLN:O	1:B:764:GLN:HG3	2.19	0.41
1:D:354:SER:HA	1:D:355:PRO:HD3	1.86	0.41
1:F:17:ILE:HG13	1:F:53:PHE:HZ	1.85	0.41
1:F:354:SER:HA	1:F:355:PRO:HD3	1.90	0.41
1:F:510:HIS:CD2	1:F:510:HIS:N	2.89	0.41
1:A:519:ALA:O	1:A:551:TYR:HE2	2.04	0.41
1:B:31:GLU:OE1	1:B:56:ARG:HD3	2.21	0.41
1:B:243:ASP:CG	1:B:244:GLY:N	2.78	0.41
1:C:145:ASN:CG	1:C:147:ARG:HG3	2.46	0.41
1:C:267:TRP:CE3	1:C:341:LYS:HG3	2.56	0.41
1:D:273:LEU:HD22	1:D:274:THR:H	1.86	0.41
1:D:276:SER:O	1:D:277:PHE:C	2.64	0.41
1:D:283:GLU:HA	1:D:331:MSE:HE1	2.02	0.41
1:F:341:LYS:O	1:F:342:ILE:HD12	2.21	0.41
1:F:745:ASN:HD22	1:F:745:ASN:N	2.19	0.41
1:B:377:TRP:NE1	1:B:379:LYS:HB2	2.36	0.40
1:B:453:LYS:HZ1	1:B:458:GLU:HG3	1.86	0.40
1:B:569:MSE:CB	1:B:573:LEU:HD22	2.51	0.40
1:B:693:LEU:HD13	1:B:693:LEU:C	2.45	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:C:199:PHE:CE2	1:C:201:MSE:HG3	2.56	0.40
1:C:306:ASP:OD2	1:C:306:ASP:C	2.64	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: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:E:609:MSE:HE2	1:E:609:MSE:CA	2.49	0.40
1:F:78:ASN:HD22	1:F:78:ASN:HA	1.70	0.40
1:A:20:LEU:HD22	1:A:134:VAL:CG2	2.50	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:E:221:GLY:HA2	1:E:224:LYS:O	2.20	0.40
1:F:312:ALA:O	1:F:313:PHE:HB2	2.19	0.40
1:A:314:GLN:HB2	1:A:354:SER:CB	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ARG:HH21	1:D:225:VAL:CG1	2.33	0.40
1:A:579:ARG:HH21	1:A:579:ARG:HG2	1.87	0.40
1:B:183:ASN:HA	1:B:196:ASN:ND2	2.36	0.40
1:E:271:LEU:O	1:E:271:LEU:HD13	2.22	0.40
1:E:309:TRP:CE2	1:E:310:MSE:HE2	2.57	0.40
1:F:408:MSE:HE2	1:F:408:MSE:HB3	1.92	0.40
1:A:19:PRO:HD2	1:A:137:ASN:OD1	2.22	0.40
1:A:381:GLN:HB2	1:A:384:LEU:HD12	2.03	0.40
1:A:475:PHE:N	1:A:476:PRO:HD3	2.36	0.40
1:A:674:ASN:HB3	1:A:680:TYR:CZ	2.57	0.40
1:A:691:PHE:O	1:A:692:ASN:C	2.63	0.40
1:B:312:ALA:O	1:B:313:PHE:HB2	2.22	0.40
1:C:39:ARG:NH2	1:C:50:THR:HB	2.37	0.40
1:C:748:GLN:HB3	1:C:769:THR:HG22	2.03	0.40
1:D:388:ASP:C	1:D:390:THR:H	2.29	0.40
1:D:754:GLU:OE2	1:D:759:LEU:HD13	2.21	0.40
1:E:326:PRO:O	1:E:328:PRO:HD3	2.21	0.40
1:E:347:ASN:HB2	1:E:348:PRO:HD2	2.03	0.40
1:E:669:LEU:HD13	1:E:670:ALA:N	2.37	0.40
1:F:195:LYS:CE	1:F:478:HIS:HB3	2.45	0.40
1:F:244:GLY:C	1:F:246:THR:N	2.78	0.40
1:F:264:PRO:HA	1:F:265:PRO:HD3	1.83	0.40
1:A:17:ILE:HG13	1:A:53:PHE:HZ	1.86	0.40
1:A:43:GLU:CG	1:A:46:TRP:CD1	3.05	0.40
1:A:377:TRP:CD1	1:A:377:TRP:C	3.00	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:D:749:ASP:HB3	1:D:764:GLN:HG3	2.03	0.40
1:E:116:GLU:CD	1:E:116:GLU:H	2.29	0.40
1:E:293:MSE:HE2	1:E:296:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	770/772 (100%)	722 (94%)	39 (5%)	9 (1%)	10	16
1	B	756/772 (98%)	702 (93%)	40 (5%)	14 (2%)	6	8
1	C	750/772 (97%)	695 (93%)	46 (6%)	9 (1%)	10	16
1	D	751/772 (97%)	700 (93%)	39 (5%)	12 (2%)	7	11
1	E	749/772 (97%)	696 (93%)	45 (6%)	8 (1%)	11	18
1	F	751/772 (97%)	703 (94%)	38 (5%)	10 (1%)	9	14
All	All	4527/4632 (98%)	4218 (93%)	247 (6%)	62 (1%)	9	13

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

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Mol	Chain	Res	Type
1	B	278	THR
1	B	316	CYS
1	B	692	ASN
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%)	617 (94%)	42 (6%)	16	28
1	B	649/640 (101%)	609 (94%)	40 (6%)	16	29
1	C	647/640 (101%)	599 (93%)	48 (7%)	13	22
1	D	647/640 (101%)	598 (92%)	49 (8%)	12	21
1	E	646/640 (101%)	601 (93%)	45 (7%)	14	24
1	F	646/640 (101%)	612 (95%)	34 (5%)	20	36
All	All	3894/3840 (101%)	3636 (93%)	258 (7%)	15	26

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	TRP
1	A	48	LEU
1	A	76	LEU
1	A	123	LEU
1	A	156	LEU
1	A	165	LEU
1	A	225	VAL
1	A	237	LEU
1	A	246	THR
1	A	263	LEU
1	A	300	LEU
1	A	316	CYS
1	A	360	LEU
1	A	367	LEU
1	A	401	LYS
1	A	402	LEU
1	A	425	VAL
1	A	447	LEU
1	A	452	LEU
1	A	453	LYS
1	A	462	VAL
1	A	463	LEU
1	A	464	PHE
1	A	466	ARG
1	A	510	HIS
1	A	517	ASN
1	A	533	LEU
1	A	537	SER

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Mol	Chain	Res	Type
1	A	573	LEU
1	A	604	LEU
1	A	653	GLN
1	A	664	ARG
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	91	LYS
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	358	LYS
1	B	367	LEU
1	B	379	LYS
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	604	LEU
1	B	619	VAL
1	B	677	ARG
1	B	681	VAL
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	738	LEU
1	B	756	GLU
1	C	41	VAL
1	C	46	TRP
1	C	47	GLN
1	C	49	ASP
1	C	76	LEU
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	374	LEU
1	C	381	GLN
1	C	390	THR
1	C	402	LEU
1	C	405	LEU
1	C	415	THR
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
1	C	537	SER

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Mol	Chain	Res	Type
1	C	539	LEU
1	C	540	HIS
1	C	575	ARG
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	686	THR
1	C	693	LEU
1	C	710	VAL
1	C	743	LYS
1	C	745	ASN
1	C	747	LEU
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	287	ASN
1	D	300	LEU
1	D	316	CYS
1	D	342	ILE
1	D	347	ASN
1	D	360	LEU
1	D	390	THR
1	D	396	LYS
1	D	402	LEU
1	D	458	GLU
1	D	459	GLU
1	D	462	VAL
1	D	463	LEU
1	D	464	PHE

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Mol	Chain	Res	Type
1	D	476	PRO
1	D	494	LEU
1	D	510	HIS
1	D	537	SER
1	D	539	LEU
1	D	540	HIS
1	D	553	ASP
1	D	573	LEU
1	D	589	ARG
1	D	592	MSE
1	D	604	LEU
1	D	619	VAL
1	D	630	LEU
1	D	638	LEU
1	D	644	LEU
1	D	684	GLU
1	D	686	THR
1	D	703	VAL
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	76	LEU
1	E	84	LEU
1	E	93	THR
1	E	108	LEU
1	E	120	LEU
1	E	123	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

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Mol	Chain	Res	Type
1	E	390	THR
1	E	452	LEU
1	E	462	VAL
1	E	463	LEU
1	E	464	PHE
1	E	476	PRO
1	E	494	LEU
1	E	502	LEU
1	E	510	HIS
1	E	537	SER
1	E	573	LEU
1	E	619	VAL
1	E	634	ARG
1	E	638	LEU
1	E	651	LYS
1	E	657	LEU
1	E	686	THR
1	E	715	LYS
1	E	718	ARG
1	E	730	GLU
1	E	733	ASN
1	E	736	LEU
1	E	738	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	156	LEU
1	F	165	LEU
1	F	248	LYS
1	F	251	LEU
1	F	271	LEU
1	F	298	LEU
1	F	316	CYS
1	F	350	ILE
1	F	360	LEU
1	F	405	LEU
1	F	463	LEU

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Mol	Chain	Res	Type
1	F	464	PHE
1	F	466	ARG
1	F	476	PRO
1	F	498	LEU
1	F	510	HIS
1	F	573	LEU
1	F	604	LEU
1	F	610	LEU
1	F	619	VAL
1	F	651	LYS
1	F	676	GLN
1	F	686	THR
1	F	693	LEU
1	F	725	VAL
1	F	726	THR
1	F	732	LYS
1	F	735	THR
1	F	743	LYS
1	F	745	ASN
1	F	747	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	18	HIS
1	A	27	GLN
1	A	88	GLN
1	A	107	ASN
1	A	125	ASN
1	A	141	GLN
1	A	144	ASN
1	A	146	GLN
1	A	192	GLN
1	A	280	ASN
1	A	439	HIS
1	A	450	ASN
1	A	517	ASN
1	A	540	HIS
1	A	613	ASN
1	A	650	HIS
1	A	653	GLN

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Mol	Chain	Res	Type
1	A	673	ASN
1	A	689	HIS
1	A	721	ASN
1	A	733	ASN
1	A	745	ASN
1	B	15	ASN
1	B	18	HIS
1	B	28	GLN
1	B	61	GLN
1	B	73	GLN
1	B	78	ASN
1	B	141	GLN
1	B	148	ASN
1	B	192	GLN
1	B	361	GLN
1	B	439	HIS
1	B	445	ASN
1	B	450	ASN
1	B	564	GLN
1	B	613	ASN
1	B	683	HIS
1	B	689	HIS
1	B	697	HIS
1	B	748	GLN
1	C	15	ASN
1	C	27	GLN
1	C	28	GLN
1	C	47	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	613	ASN
1	C	627	GLN
1	C	653	GLN

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Mol	Chain	Res	Type
1	C	673	ASN
1	C	683	HIS
1	C	697	HIS
1	C	721	ASN
1	C	733	ASN
1	C	745	ASN
1	C	752	GLN
1	C	766	ASN
1	D	28	GLN
1	D	71	HIS
1	D	88	GLN
1	D	347	ASN
1	D	434	GLN
1	D	439	HIS
1	D	540	HIS
1	D	564	GLN
1	D	627	GLN
1	D	697	HIS
1	D	733	ASN
1	D	745	ASN
1	D	748	GLN
1	D	752	GLN
1	D	757	GLN
1	E	27	GLN
1	E	28	GLN
1	E	73	GLN
1	E	78	ASN
1	E	88	GLN
1	E	107	ASN
1	E	125	ASN
1	E	141	GLN
1	E	146	GLN
1	E	148	ASN
1	E	280	ASN
1	E	287	ASN
1	E	347	ASN
1	E	361	GLN
1	E	613	ASN
1	E	666	ASN
1	E	676	GLN
1	E	694	GLN
1	E	721	ASN

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Mol	Chain	Res	Type
1	E	733	ASN
1	E	745	ASN
1	E	748	GLN
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	445	ASN
1	F	564	GLN
1	F	613	ASN
1	F	627	GLN
1	F	676	GLN
1	F	692	ASN
1	F	697	HIS
1	F	740	ASN
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 oligosaccharides 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	B	802	-	12,12,12	0.52	0	15,16,16	0.70	0
2	MES	C	803	-	12,12,12	0.50	0	15,16,16	0.71	0
2	MES	E	805	-	12,12,12	0.51	0	15,16,16	0.65	0
2	MES	A	801	-	12,12,12	0.61	0	15,16,16	0.80	0
2	MES	D	804	-	12,12,12	0.52	0	15,16,16	0.76	0
2	MES	F	806	-	12,12,12	0.44	0	15,16,16	0.91	1 (6%)

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	B	802	-	-	3/6/14/14	0/1/1/1
2	MES	C	803	-	-	3/6/14/14	0/1/1/1
2	MES	E	805	-	-	2/6/14/14	0/1/1/1
2	MES	A	801	-	-	3/6/14/14	0/1/1/1
2	MES	D	804	-	-	6/6/14/14	0/1/1/1
2	MES	F	806	-	-	5/6/14/14	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	806	MES	O1S-S-C8	-2.06	103.61	106.73

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	802	MES	C7-C8-S-O2S
2	B	802	MES	C7-C8-S-O3S
2	C	803	MES	C7-C8-S-O2S
2	C	803	MES	C7-C8-S-O3S
2	D	804	MES	N4-C7-C8-S
2	D	804	MES	C7-C8-S-O1S
2	D	804	MES	C7-C8-S-O3S

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Mol	Chain	Res	Type	Atoms
2	E	805	MES	C8-C7-N4-C3
2	E	805	MES	C8-C7-N4-C5
2	F	806	MES	C7-C8-S-O1S
2	F	806	MES	C7-C8-S-O2S
2	A	801	MES	C7-C8-S-O3S
2	D	804	MES	C8-C7-N4-C3
2	F	806	MES	C8-C7-N4-C5
2	F	806	MES	C7-C8-S-O3S
2	A	801	MES	C7-C8-S-O1S
2	A	801	MES	C7-C8-S-O2S
2	B	802	MES	C7-C8-S-O1S
2	C	803	MES	C7-C8-S-O1S
2	D	804	MES	C7-C8-S-O2S
2	D	804	MES	C8-C7-N4-C5
2	F	806	MES	C8-C7-N4-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	803	MES	2	0
2	E	805	MES	1	0
2	A	801	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%)	0.08	22 (2%)	53	50	29, 45, 79, 101	0
1	B	741/772 (95%)	0.15	30 (4%)	42	38	31, 45, 86, 102	0
1	C	737/772 (95%)	0.03	23 (3%)	51	47	30, 43, 75, 95	0
1	D	738/772 (95%)	-0.01	14 (1%)	66	62	29, 42, 75, 100	0
1	E	736/772 (95%)	0.22	33 (4%)	38	34	31, 47, 79, 99	0
1	F	738/772 (95%)	0.14	22 (2%)	52	48	32, 48, 82, 100	0
All	All	4443/4632 (95%)	0.10	144 (3%)	50	46	29, 45, 79, 102	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	772	LEU	7.2
1	F	314	GLN	6.4
1	F	244	GLY	6.2
1	B	41	VAL	6.2
1	B	768	LEU	6.0
1	B	767	ALA	5.7
1	A	244	GLY	5.7
1	D	319	GLU	5.6
1	B	244	GLY	5.6
1	C	300	LEU	5.4
1	D	765	GLY	5.3
1	B	46	TRP	5.1
1	C	287	ASN	5.0
1	D	767	ALA	4.6
1	C	46	TRP	4.3
1	B	286	VAL	4.2
1	F	344	VAL	4.1
1	E	519	ALA	4.1
1	B	302	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	682	TRP	4.0
1	C	767	ALA	3.6
1	E	767	ALA	3.6
1	A	745	ASN	3.6
1	B	613	ASN	3.6
1	E	711	ILE	3.5
1	E	765	GLY	3.5
1	C	275	THR	3.5
1	B	416	ASP	3.4
1	F	505	PHE	3.4
1	C	298	LEU	3.4
1	F	458	GLU	3.4
1	E	79	GLY	3.4
1	D	394	ALA	3.4
1	C	280	ASN	3.3
1	A	516	GLU	3.3
1	C	771	THR	3.2
1	F	513	GLY	3.2
1	D	624	GLY	3.1
1	E	127	GLU	3.1
1	D	766	ASN	3.1
1	E	296	ARG	3.1
1	A	543	LYS	3.0
1	E	484	TYR	3.0
1	A	46	TRP	3.0
1	A	315	TRP	3.0
1	E	316	CYS	3.0
1	B	757	GLN	3.0
1	E	448	VAL	2.9
1	E	512	ILE	2.9
1	D	46	TRP	2.9
1	E	452	LEU	2.9
1	F	752	GLN	2.9
1	C	297	ASN	2.9
1	A	26	GLU	2.9
1	A	540	HIS	2.9
1	B	657	LEU	2.9
1	B	243	ASP	2.9
1	B	288	SER	2.9
1	C	244	GLY	2.9
1	F	765	GLY	2.9
1	F	315	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	145	ASN	2.8
1	E	49	ASP	2.8
1	E	676	GLN	2.8
1	E	752	GLN	2.8
1	A	515	PHE	2.8
1	A	113	SER	2.8
1	B	29	ASP	2.8
1	C	530	PHE	2.8
1	D	696	GLY	2.8
1	D	753	ALA	2.7
1	C	276	SER	2.7
1	A	541	GLY	2.7
1	F	759	LEU	2.7
1	F	504	GLY	2.7
1	F	280	ASN	2.7
1	C	26	GLU	2.7
1	E	479	TRP	2.6
1	E	748	GLN	2.6
1	C	484	TYR	2.6
1	E	60	PRO	2.6
1	F	281	TYR	2.6
1	B	317	ASP	2.6
1	B	514	GLY	2.5
1	F	753	ALA	2.5
1	E	278	THR	2.5
1	E	281	TYR	2.5
1	E	291	ASP	2.5
1	A	765	GLY	2.5
1	B	89	ASP	2.5
1	C	730	GLU	2.5
1	D	659	LEU	2.5
1	C	518	THR	2.5
1	D	740	ASN	2.5
1	E	485	ALA	2.5
1	D	276	SER	2.5
1	E	751	SER	2.5
1	C	720	GLY	2.4
1	E	383	GLY	2.4
1	F	729	GLY	2.4
1	F	79	GLY	2.4
1	A	380	TRP	2.4
1	A	518	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	769	THR	2.4
1	A	333	ARG	2.4
1	E	764	GLN	2.4
1	C	278	THR	2.3
1	A	517	ASN	2.3
1	C	770	ILE	2.3
1	C	30	ASN	2.3
1	F	745	ASN	2.3
1	B	301	HIS	2.3
1	C	459	GLU	2.3
1	C	45	THR	2.2
1	B	754	GLU	2.2
1	B	747	LEU	2.2
1	B	380	TRP	2.2
1	F	350	ILE	2.2
1	E	456	VAL	2.2
1	F	577	ALA	2.2
1	A	696	GLY	2.2
1	E	555	SER	2.2
1	B	43	GLU	2.2
1	E	280	ASN	2.1
1	B	758	GLY	2.1
1	C	277	PHE	2.1
1	E	577	ALA	2.1
1	A	697	HIS	2.1
1	D	381	GLN	2.1
1	A	768	LEU	2.1
1	B	284	ALA	2.1
1	B	519	ALA	2.1
1	B	766	ASN	2.1
1	E	538	ARG	2.1
1	E	431	SER	2.1
1	F	469	SER	2.1
1	F	477	VAL	2.0
1	B	517	ASN	2.0
1	A	393	ASP	2.0
1	E	509	SER	2.0
1	A	458	GLU	2.0
1	E	116	GLU	2.0
1	F	750	GLY	2.0
1	B	299	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MES	A	801	12/12	0.71	0.22	81,82,83,83	0
2	MES	E	805	12/12	0.76	0.20	79,80,81,81	0
2	MES	C	803	12/12	0.81	0.15	54,59,60,62	0
2	MES	B	802	12/12	0.84	0.15	81,85,86,87	0
2	MES	D	804	12/12	0.90	0.12	56,64,67,68	0
2	MES	F	806	12/12	0.90	0.13	67,73,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.