



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 04:43 AM EDT

PDB ID : 3MSY  
Title : Crystal Structure of Mandelate racemase/muconate lactonizing enzyme from a Marine actinobacterium  
Authors : Satyanarayana, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2010-04-29  
Resolution : 2.50 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

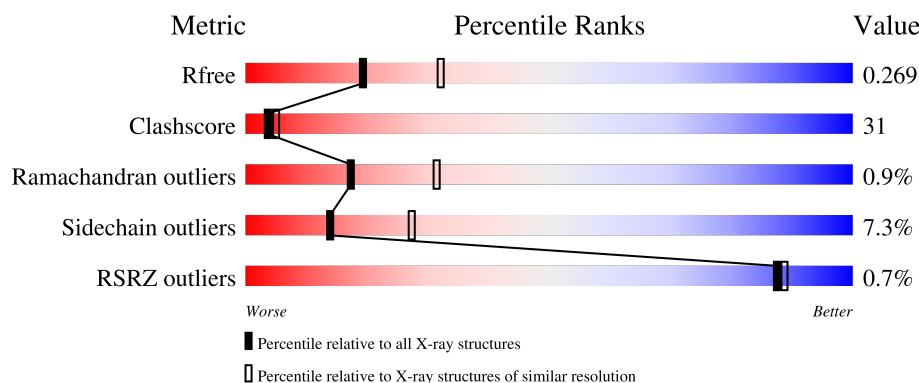
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	379	
1	B	379	
1	C	379	
1	D	379	
1	E	379	

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Mol	Chain	Length	Quality of chain
1	F	379	<div><div><div>%</div><div><div></div></div><div>53%</div><div>36%</div><div>• 7%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16869 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 Mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	Se	0	0	0
			2731	1723	481	512	5	10			
1	B	351	Total	C	N	O	S	Se	0	0	0
			2747	1732	485	515	5	10			
1	C	355	Total	C	N	O	S	Se	0	0	0
			2786	1757	493	521	5	10			
1	D	351	Total	C	N	O	S	Se	0	0	0
			2747	1732	485	515	5	10			
1	E	350	Total	C	N	O	S	Se	0	0	0
			2737	1726	482	514	5	10			
1	F	351	Total	C	N	O	S	Se	0	0	0
			2747	1732	485	515	5	10			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MSE	-	expression tag	UNP A4AFX2
A	19	SER	-	expression tag	UNP A4AFX2
A	389	GLU	-	expression tag	UNP A4AFX2
A	390	GLY	-	expression tag	UNP A4AFX2
A	391	HIS	-	expression tag	UNP A4AFX2
A	392	HIS	-	expression tag	UNP A4AFX2
A	393	HIS	-	expression tag	UNP A4AFX2
A	394	HIS	-	expression tag	UNP A4AFX2
A	395	HIS	-	expression tag	UNP A4AFX2
A	396	HIS	-	expression tag	UNP A4AFX2
B	18	MSE	-	expression tag	UNP A4AFX2
B	19	SER	-	expression tag	UNP A4AFX2
B	389	GLU	-	expression tag	UNP A4AFX2
B	390	GLY	-	expression tag	UNP A4AFX2
B	391	HIS	-	expression tag	UNP A4AFX2
B	392	HIS	-	expression tag	UNP A4AFX2
B	393	HIS	-	expression tag	UNP A4AFX2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	394	HIS	-	expression tag	UNP A4AFX2
B	395	HIS	-	expression tag	UNP A4AFX2
B	396	HIS	-	expression tag	UNP A4AFX2
C	18	MSE	-	expression tag	UNP A4AFX2
C	19	SER	-	expression tag	UNP A4AFX2
C	389	GLU	-	expression tag	UNP A4AFX2
C	390	GLY	-	expression tag	UNP A4AFX2
C	391	HIS	-	expression tag	UNP A4AFX2
C	392	HIS	-	expression tag	UNP A4AFX2
C	393	HIS	-	expression tag	UNP A4AFX2
C	394	HIS	-	expression tag	UNP A4AFX2
C	395	HIS	-	expression tag	UNP A4AFX2
C	396	HIS	-	expression tag	UNP A4AFX2
D	18	MSE	-	expression tag	UNP A4AFX2
D	19	SER	-	expression tag	UNP A4AFX2
D	389	GLU	-	expression tag	UNP A4AFX2
D	390	GLY	-	expression tag	UNP A4AFX2
D	391	HIS	-	expression tag	UNP A4AFX2
D	392	HIS	-	expression tag	UNP A4AFX2
D	393	HIS	-	expression tag	UNP A4AFX2
D	394	HIS	-	expression tag	UNP A4AFX2
D	395	HIS	-	expression tag	UNP A4AFX2
D	396	HIS	-	expression tag	UNP A4AFX2
E	18	MSE	-	expression tag	UNP A4AFX2
E	19	SER	-	expression tag	UNP A4AFX2
E	389	GLU	-	expression tag	UNP A4AFX2
E	390	GLY	-	expression tag	UNP A4AFX2
E	391	HIS	-	expression tag	UNP A4AFX2
E	392	HIS	-	expression tag	UNP A4AFX2
E	393	HIS	-	expression tag	UNP A4AFX2
E	394	HIS	-	expression tag	UNP A4AFX2
E	395	HIS	-	expression tag	UNP A4AFX2
E	396	HIS	-	expression tag	UNP A4AFX2
F	18	MSE	-	expression tag	UNP A4AFX2
F	19	SER	-	expression tag	UNP A4AFX2
F	389	GLU	-	expression tag	UNP A4AFX2
F	390	GLY	-	expression tag	UNP A4AFX2
F	391	HIS	-	expression tag	UNP A4AFX2
F	392	HIS	-	expression tag	UNP A4AFX2
F	393	HIS	-	expression tag	UNP A4AFX2
F	394	HIS	-	expression tag	UNP A4AFX2
F	395	HIS	-	expression tag	UNP A4AFX2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	396	HIS	-	expression tag	UNP A4AFX2

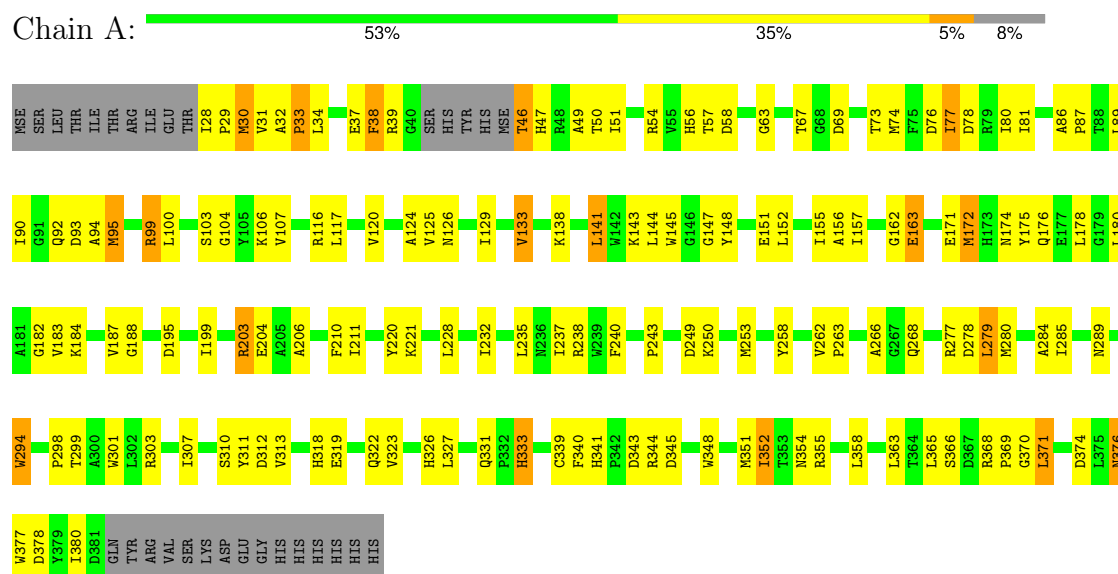
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	65	Total O 65 65	0	0
2	B	62	Total O 62 62	0	0
2	C	63	Total O 63 63	0	0
2	D	72	Total O 72 72	0	0
2	E	55	Total O 55 55	0	0
2	F	57	Total O 57 57	0	0

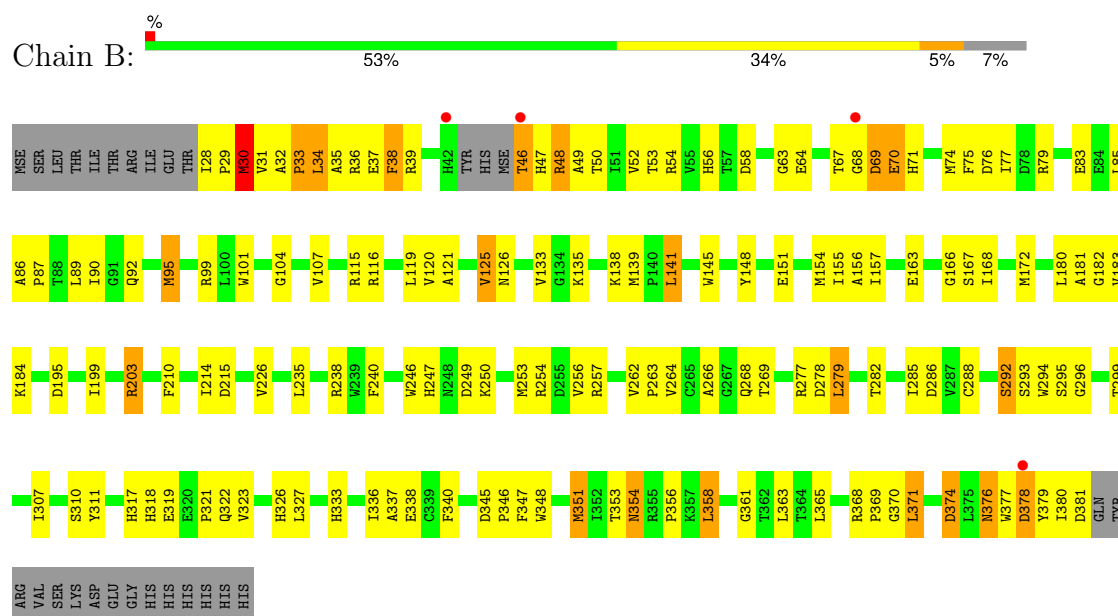
### 3 Residue-property plots

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: Mandelate racemase/muconate lactonizing enzyme

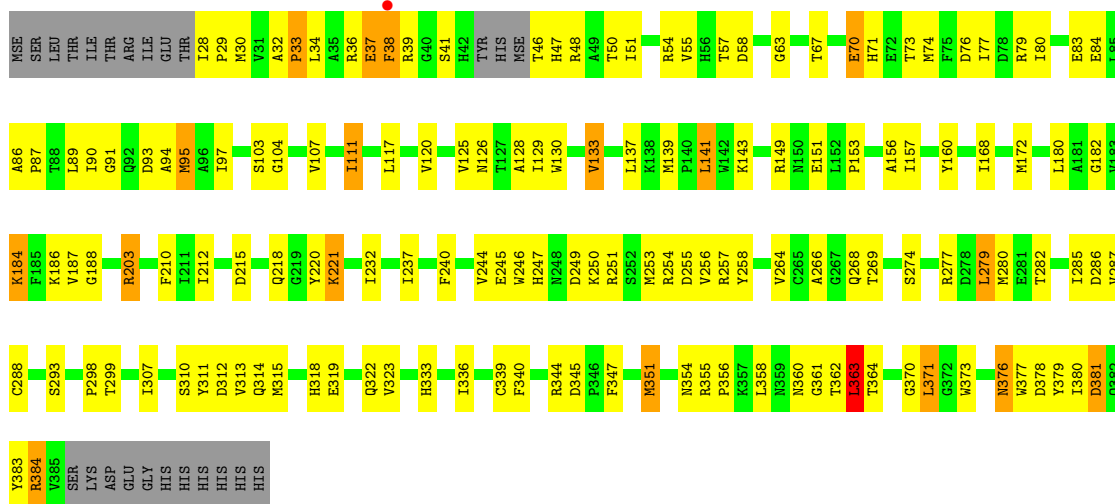


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



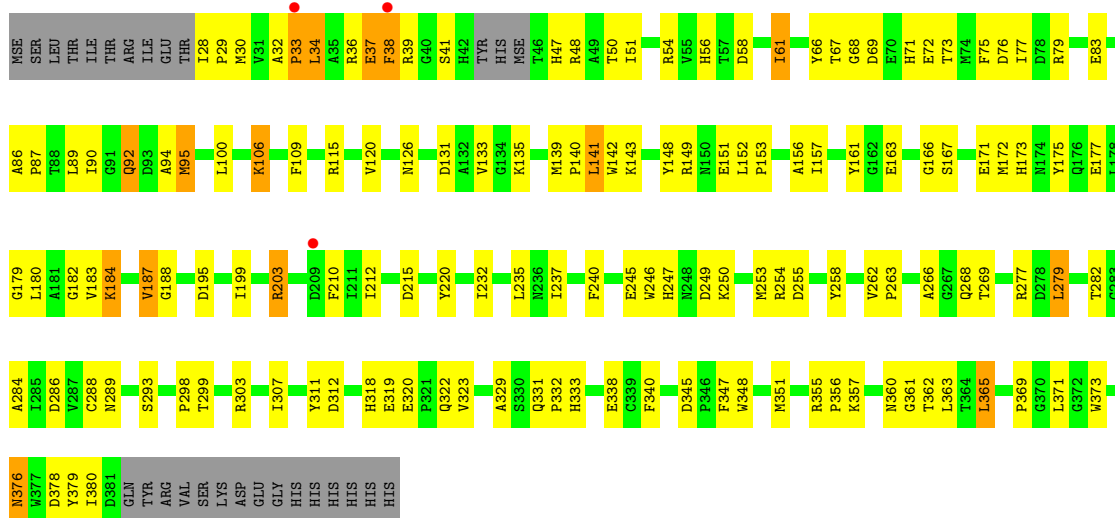
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain C: 



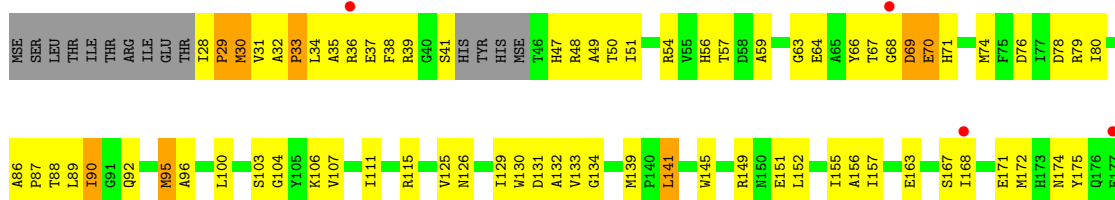
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain D: 

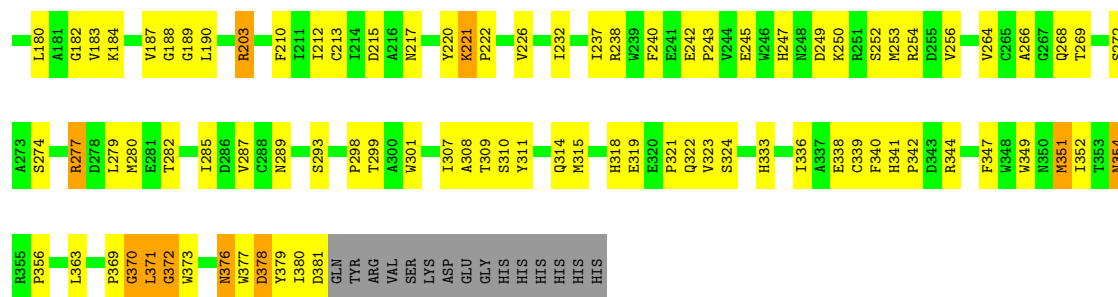


• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

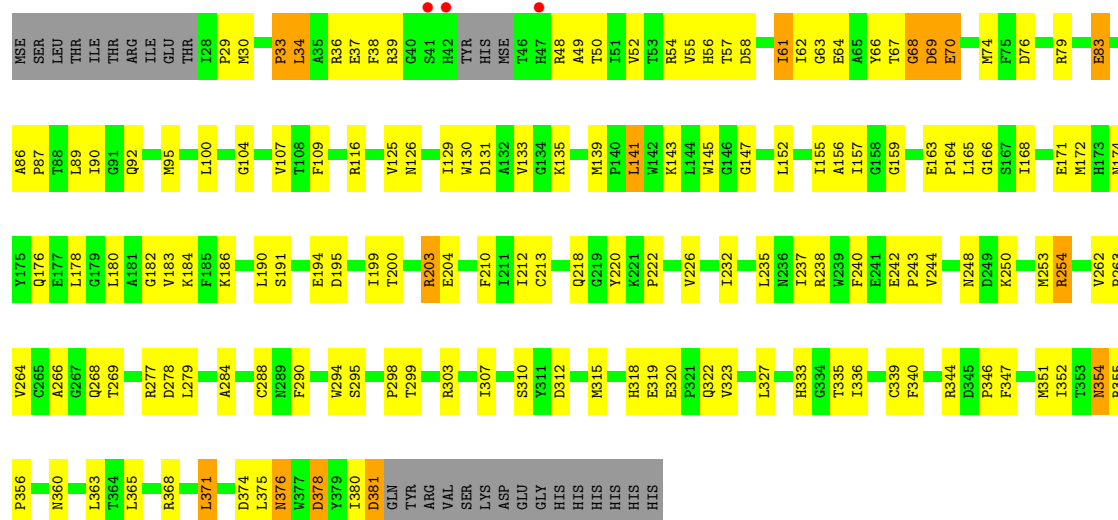
Chain E: 







- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.00Å 103.39Å 234.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.31 – 2.50 47.31 – 2.22	Depositor EDS
% Data completeness (in resolution range)	94.6 (47.31-2.50) 96.0 (47.31-2.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.76	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.238 , 0.268 0.225 , 0.269	Depositor DCC
$R_{free}$ test set	5679 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16869	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.38	0/2790	0.67	0/3779
1	B	0.38	0/2807	0.67	1/3802 (0.0%)
1	C	0.38	0/2847	0.67	1/3856 (0.0%)
1	D	0.38	0/2807	0.68	0/3802
1	E	0.37	0/2796	0.69	0/3787
1	F	0.36	0/2807	0.65	1/3802 (0.0%)
All	All	0.37	0/16854	0.67	3/22828 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	68	GLY	N-CA-C	6.79	130.08	113.10
1	B	30	MSE	CB-CG-SE	-5.69	95.63	112.70
1	C	363	LEU	CA-CB-CG	5.17	127.19	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2731	0	2624	170	0
1	B	2747	0	2636	183	0
1	C	2786	0	2675	200	0
1	D	2747	0	2636	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2737	0	2629	208	0
1	F	2747	0	2636	151	0
2	A	65	0	0	19	0
2	B	62	0	0	14	0
2	C	63	0	0	16	0
2	D	72	0	0	6	0
2	E	55	0	0	30	0
2	F	57	0	0	9	0
All	All	16869	0	15836	1015	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 31.

All (1015) 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:376:ASN:HD21	1:E:378:ASP:HB2	1.16	1.06
1:D:67:THR:HG23	1:D:293:SER:HB2	1.36	1.05
1:E:30:MSE:HE2	1:E:89:LEU:HB3	1.35	1.03
1:C:253:MSE:HE3	1:C:264:VAL:HG12	1.42	1.00
1:C:37:GLU:H	1:C:37:GLU:CD	1.66	0.99
1:D:351:MSE:HE1	1:D:380:ILE:HG13	1.44	0.98
1:A:374:ASP:HB2	2:A:433:HOH:O	1.63	0.97
1:B:253:MSE:HE3	1:B:264:VAL:CG1	1.95	0.97
1:E:51:ILE:HD13	2:E:434:HOH:O	1.63	0.96
1:A:351:MSE:HE3	1:A:380:ILE:HG12	1.45	0.96
1:D:268:GLN:HE21	1:D:289:ASN:HD21	1.09	0.96
1:E:95:MSE:HB3	1:F:143:LYS:HD3	1.45	0.96
1:F:243:PRO:HD2	1:F:253:MSE:HE3	1.50	0.94
1:B:253:MSE:HE3	1:B:264:VAL:HG12	1.50	0.93
1:A:99:ARG:HH11	1:A:99:ARG:HG3	1.34	0.93
1:E:371:LEU:HD11	1:E:373:TRP:CD1	2.04	0.93
1:D:277:ARG:HG2	2:D:433:HOH:O	1.68	0.93
1:E:253:MSE:HE3	1:E:264:VAL:CG1	1.99	0.93
1:E:371:LEU:HD12	1:E:372:GLY:H	1.34	0.92
1:A:277:ARG:HG2	1:A:277:ARG:HH11	1.33	0.92
1:B:70:GLU:HG3	1:B:77:ILE:HD12	1.49	0.92
1:C:253:MSE:HE3	1:C:264:VAL:CG1	2.01	0.91
1:B:156:ALA:HB2	1:B:180:LEU:HD13	1.49	0.91
1:A:310:SER:HB2	2:A:454:HOH:O	1.71	0.90
1:C:153:PRO:HG2	1:C:336:ILE:HG22	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:MSE:HG3	1:C:90:ILE:HA	1.52	0.90
1:C:34:LEU:HD23	1:C:54:ARG:HD3	1.53	0.89
1:F:141:LEU:HD23	1:F:371:LEU:HD13	1.55	0.87
1:D:347:PHE:O	1:D:351:MSE:HB2	1.73	0.87
1:D:33:PRO:HD3	1:D:90:ILE:HD11	1.55	0.87
1:A:156:ALA:HB2	1:A:180:LEU:HD13	1.56	0.87
1:B:253:MSE:HA	1:B:256:VAL:HG12	1.57	0.87
1:C:376:ASN:ND2	1:C:379:TYR:H	1.73	0.87
1:A:141:LEU:HD23	1:A:371:LEU:HD13	1.55	0.86
1:C:186:LYS:HE2	2:C:441:HOH:O	1.76	0.86
1:A:253:MSE:HE1	1:A:285:ILE:CG2	2.06	0.85
1:D:277:ARG:HG2	1:D:277:ARG:HH11	1.40	0.84
1:E:371:LEU:HD11	1:E:373:TRP:NE1	1.92	0.84
1:F:33:PRO:HD3	1:F:90:ILE:HD11	1.57	0.84
1:C:34:LEU:HD23	1:C:54:ARG:HH11	1.43	0.83
1:F:34:LEU:HB3	2:F:418:HOH:O	1.77	0.83
1:C:376:ASN:C	1:C:376:ASN:HD22	1.80	0.83
1:F:30:MSE:HB2	2:F:428:HOH:O	1.78	0.83
1:E:277:ARG:HA	1:E:280:MSE:HE3	1.60	0.82
1:E:371:LEU:HD13	2:E:429:HOH:O	1.79	0.82
1:A:29:PRO:HD2	1:A:58:ASP:CG	1.99	0.82
1:C:254:ARG:HG2	1:C:254:ARG:HH11	1.44	0.82
1:C:156:ALA:HB2	1:C:180:LEU:HD13	1.61	0.82
1:C:30:MSE:CG	1:C:90:ILE:HA	2.08	0.81
1:C:50:THR:HG22	1:C:347:PHE:HE2	1.44	0.81
1:F:277:ARG:HH11	1:F:277:ARG:HG2	1.45	0.81
1:A:376:ASN:HD21	1:A:378:ASP:HB2	1.44	0.81
1:E:376:ASN:ND2	1:E:378:ASP:HB2	1.95	0.81
1:B:184:LYS:HD3	1:B:215:ASP:HB2	1.62	0.81
1:D:254:ARG:HD3	1:D:282:THR:O	1.80	0.81
1:A:232:ILE:HD12	1:A:237:ILE:HG13	1.64	0.80
1:E:89:LEU:HD11	1:E:125:VAL:HG11	1.63	0.80
1:C:253:MSE:HA	1:C:256:VAL:HG12	1.64	0.80
1:C:277:ARG:HG2	1:C:277:ARG:HH11	1.45	0.80
1:B:354:ASN:HD22	1:B:354:ASN:H	1.28	0.79
1:E:38:PHE:CZ	1:E:380:ILE:HG13	2.17	0.79
1:E:253:MSE:HE3	1:E:264:VAL:HG11	1.64	0.79
1:E:266:ALA:HB2	2:E:450:HOH:O	1.82	0.79
1:D:41:SER:HA	1:D:47:HIS:ND1	1.97	0.78
1:E:41:SER:HB3	1:E:47:HIS:ND1	1.98	0.78
1:F:347:PHE:O	1:F:351:MSE:HB2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LEU:HD11	1:C:125:VAL:HG11	1.64	0.78
1:E:351:MSE:HE3	1:E:379:TYR:HD2	1.48	0.77
1:D:48:ARG:HD2	1:D:69:ASP:OD2	1.83	0.77
1:C:38:PHE:HB3	1:C:384:ARG:HA	1.65	0.77
1:C:30:MSE:HG2	1:C:89:LEU:C	2.04	0.76
1:E:70:GLU:HB2	2:E:423:HOH:O	1.84	0.76
1:E:253:MSE:HE3	1:E:264:VAL:HG12	1.66	0.76
1:E:37:GLU:H	1:E:37:GLU:CD	1.84	0.76
1:F:354:ASN:HD22	1:F:354:ASN:H	1.30	0.76
1:E:88:THR:HG21	2:E:414:HOH:O	1.86	0.76
1:D:38:PHE:CE2	1:D:380:ILE:HG12	2.20	0.76
1:F:322:GLN:HG2	1:F:323:VAL:HG23	1.66	0.76
1:B:254:ARG:HG2	1:B:254:ARG:HH11	1.50	0.75
1:B:351:MSE:HE1	1:B:380:ILE:HG12	1.68	0.75
1:B:67:THR:HG23	1:B:293:SER:OG	1.86	0.75
1:B:163:GLU:HB3	1:B:166:GLY:O	1.86	0.75
1:E:371:LEU:CD1	1:E:372:GLY:H	2.00	0.74
1:C:104:GLY:HA3	2:C:411:HOH:O	1.86	0.74
1:B:70:GLU:HG3	1:B:77:ILE:CD1	2.18	0.74
1:C:254:ARG:HD3	1:C:282:THR:O	1.87	0.74
1:B:141:LEU:HD23	1:B:371:LEU:HD13	1.70	0.74
1:E:311:TYR:CZ	1:F:277:ARG:HD2	2.23	0.74
1:A:174:ASN:O	1:A:178:LEU:HG	1.88	0.73
1:F:243:PRO:HD2	1:F:253:MSE:CE	2.17	0.73
1:F:61:ILE:HD12	1:F:62:ILE:N	2.04	0.73
1:F:49:ALA:O	1:F:69:ASP:HA	1.88	0.73
1:E:253:MSE:HE1	1:E:285:ILE:HG22	1.71	0.73
1:A:67:THR:HG22	2:A:436:HOH:O	1.89	0.73
1:D:250:LYS:HG2	1:D:279:LEU:HD22	1.70	0.73
1:D:268:GLN:HE21	1:D:289:ASN:ND2	1.86	0.73
1:E:36:ARG:NH1	1:E:377:TRP:HE1	1.85	0.73
1:A:253:MSE:CE	1:A:285:ILE:HG23	2.17	0.72
1:A:352:ILE:HD12	1:A:354:ASN:H	1.52	0.72
1:D:303:ARG:O	1:D:307:ILE:HG12	1.89	0.72
1:D:268:GLN:NE2	1:D:289:ASN:HD21	1.86	0.72
1:A:253:MSE:HE1	1:A:285:ILE:HG22	1.69	0.72
1:D:254:ARG:HG2	1:D:254:ARG:HH11	1.55	0.72
1:F:50:THR:H	1:F:74:MSE:HE1	1.53	0.72
1:B:354:ASN:HD21	1:B:374:ASP:H	1.38	0.72
1:F:156:ALA:HB2	1:F:180:LEU:HD13	1.71	0.72
1:C:311:TYR:CE2	1:D:277:ARG:HD2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:MSE:HE3	1:A:380:ILE:CG1	2.18	0.71
1:D:37:GLU:CD	1:D:37:GLU:H	1.93	0.71
1:B:253:MSE:HE3	1:B:264:VAL:HG11	1.71	0.71
1:F:34:LEU:HD23	1:F:56:HIS:NE2	2.05	0.71
1:A:89:LEU:HD11	1:A:125:VAL:HG11	1.72	0.71
1:C:141:LEU:HD23	1:C:371:LEU:HD13	1.71	0.71
1:A:358:LEU:HD23	2:A:451:HOH:O	1.90	0.71
1:B:253:MSE:HE2	1:B:285:ILE:HG22	1.71	0.71
1:B:377:TRP:CE3	1:B:380:ILE:HD12	2.25	0.71
1:B:30:MSE:HB3	1:B:90:ILE:HA	1.71	0.71
1:C:287:VAL:HG22	1:C:314:GLN:HB2	1.72	0.70
1:E:36:ARG:HH11	1:E:377:TRP:HE1	1.36	0.70
1:E:372:GLY:N	2:E:429:HOH:O	2.22	0.70
1:A:249:ASP:O	1:A:253:MSE:HG2	1.91	0.70
1:B:50:THR:N	1:B:74:MSE:HE1	2.06	0.70
1:E:50:THR:H	1:E:74:MSE:HE1	1.57	0.70
1:E:126:ASN:HD21	1:E:299:THR:H	1.38	0.70
1:A:33:PRO:HD3	1:A:90:ILE:HD11	1.74	0.70
1:E:76:ASP:HA	1:E:79:ARG:HH12	1.56	0.70
1:A:277:ARG:HD2	1:B:311:TYR:CZ	2.27	0.70
1:E:254:ARG:HG2	1:E:254:ARG:HH11	1.56	0.70
1:B:253:MSE:CE	1:B:285:ILE:HG22	2.21	0.69
1:A:253:MSE:CE	1:A:285:ILE:CG2	2.70	0.69
1:B:356:PRO:HG2	1:B:363:LEU:HD11	1.74	0.69
1:B:254:ARG:HD3	1:B:282:THR:O	1.92	0.69
1:E:139:MSE:O	1:E:370:GLY:N	2.22	0.69
1:F:253:MSE:HG2	1:F:284:ALA:HB1	1.73	0.69
1:C:354:ASN:HA	2:C:457:HOH:O	1.92	0.69
1:F:37:GLU:N	1:F:37:GLU:OE2	2.25	0.69
1:A:29:PRO:HA	1:A:92:GLN:O	1.93	0.69
1:E:203:ARG:HG2	1:E:212:ILE:HD12	1.73	0.69
1:A:352:ILE:N	2:A:450:HOH:O	2.26	0.69
1:D:356:PRO:HG2	1:D:363:LEU:HD11	1.74	0.69
1:F:190:LEU:HB3	1:F:194:GLU:OE1	1.93	0.69
1:E:376:ASN:ND2	1:E:378:ASP:H	1.90	0.69
1:D:126:ASN:HD22	1:D:298:PRO:HD2	1.57	0.68
1:E:131:ASP:HA	2:E:431:HOH:O	1.92	0.68
1:A:358:LEU:HA	2:A:451:HOH:O	1.93	0.68
1:A:352:ILE:HD11	1:A:355:ARG:N	2.08	0.68
1:C:141:LEU:HD22	1:C:370:GLY:HA2	1.75	0.68
1:C:253:MSE:CE	1:C:285:ILE:HG22	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ARG:NH2	2:A:433:HOH:O	2.25	0.68
1:E:67:THR:HG23	1:E:293:SER:HB3	1.75	0.68
1:B:277:ARG:NE	2:B:412:HOH:O	2.25	0.68
1:C:253:MSE:SE	2:C:413:HOH:O	2.62	0.68
1:A:280:MSE:HG2	1:A:313:VAL:HG21	1.76	0.68
1:B:79:ARG:HG2	1:B:83:GLU:OE1	1.93	0.68
1:A:352:ILE:HG13	1:A:355:ARG:HG3	1.76	0.68
1:E:253:MSE:CE	1:E:285:ILE:HG22	2.24	0.68
1:B:50:THR:H	1:B:74:MSE:HE1	1.59	0.67
1:B:157:ILE:HG12	1:B:184:LYS:HE2	1.76	0.67
1:C:28:ILE:HG23	1:C:94:ALA:HB3	1.74	0.67
1:D:29:PRO:HD2	1:D:58:ASP:OD2	1.95	0.67
1:B:48:ARG:HH21	1:B:347:PHE:HD2	1.41	0.67
1:E:80:ILE:HG12	2:E:413:HOH:O	1.95	0.67
1:F:70:GLU:CD	1:F:70:GLU:H	1.98	0.67
1:A:268:GLN:NE2	2:A:431:HOH:O	2.26	0.67
1:D:126:ASN:HD21	1:D:299:THR:H	1.43	0.67
1:D:149:ARG:HD2	1:D:151:GLU:O	1.95	0.67
1:D:340:PHE:HB2	1:D:345:ASP:HB3	1.75	0.67
1:E:126:ASN:HD22	1:E:298:PRO:HD2	1.60	0.67
1:E:222:PRO:O	1:E:226:VAL:HG23	1.94	0.67
1:B:277:ARG:HG2	1:B:277:ARG:HH11	1.59	0.67
1:F:253:MSE:HE2	1:F:264:VAL:CG1	2.25	0.67
1:C:126:ASN:HD21	1:C:299:THR:H	1.43	0.66
1:E:36:ARG:NH1	1:E:377:TRP:NE1	2.44	0.66
1:B:101:TRP:HZ3	1:B:296:GLY:O	1.79	0.66
1:E:376:ASN:HD21	1:E:378:ASP:CB	2.03	0.66
1:F:30:MSE:CB	2:F:428:HOH:O	2.40	0.66
1:C:111:ILE:O	1:C:111:ILE:HD13	1.96	0.65
1:F:61:ILE:HD11	1:F:135:LYS:HD2	1.77	0.65
1:F:86:ALA:HB3	1:F:87:PRO:HD3	1.78	0.65
1:D:34:LEU:HD23	1:D:56:HIS:NE2	2.12	0.65
1:F:298:PRO:HB3	1:F:327:LEU:HD21	1.77	0.65
1:D:38:PHE:HE2	1:D:380:ILE:HG12	1.59	0.65
1:C:28:ILE:HD11	1:C:57:THR:HG21	1.79	0.65
1:F:50:THR:N	1:F:74:MSE:HE1	2.11	0.65
1:E:242:GLU:HA	2:E:450:HOH:O	1.95	0.65
1:C:277:ARG:HD2	1:D:311:TYR:CZ	2.31	0.65
1:B:33:PRO:HD3	1:B:90:ILE:HD11	1.79	0.65
1:C:95:MSE:CG	1:D:139:MSE:HE1	2.27	0.65
1:A:331:GLN:HB3	1:A:333:HIS:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:MSE:HG2	1:C:313:VAL:HG21	1.79	0.64
1:D:351:MSE:HE3	1:D:379:TYR:HD2	1.60	0.64
1:F:61:ILE:HD12	1:F:62:ILE:H	1.60	0.64
1:B:253:MSE:HE2	1:B:285:ILE:CG2	2.27	0.64
1:A:34:LEU:HD23	1:A:54:ARG:HD3	1.78	0.64
1:C:315:MSE:SE	2:C:422:HOH:O	2.64	0.64
1:F:33:PRO:HD3	1:F:90:ILE:CD1	2.26	0.64
1:A:363:LEU:HA	2:A:451:HOH:O	1.98	0.64
1:E:38:PHE:HZ	1:E:380:ILE:HG13	1.61	0.64
1:E:232:ILE:HD12	1:E:237:ILE:HG13	1.78	0.64
1:E:376:ASN:C	1:E:376:ASN:HD22	1.98	0.64
1:D:29:PRO:HA	1:D:92:GLN:O	1.97	0.64
1:D:50:THR:HG22	1:D:347:PHE:HE2	1.62	0.64
1:A:250:LYS:HG2	1:A:279:LEU:HD13	1.78	0.63
1:E:37:GLU:C	1:E:38:PHE:HD2	2.02	0.63
1:C:95:MSE:HG3	1:D:139:MSE:HE1	1.81	0.63
1:C:253:MSE:HE2	1:C:285:ILE:HG22	1.79	0.63
1:C:376:ASN:HD21	1:C:379:TYR:H	1.46	0.63
1:D:250:LYS:HG2	1:D:279:LEU:CD2	2.28	0.63
1:D:322:GLN:HG2	1:D:323:VAL:HG23	1.80	0.63
1:E:76:ASP:HA	1:E:79:ARG:NH1	2.12	0.63
1:E:333:HIS:CD2	2:E:443:HOH:O	2.50	0.63
1:E:344:ARG:HG3	1:E:344:ARG:HH11	1.64	0.63
1:C:37:GLU:CD	1:C:37:GLU:N	2.43	0.63
1:F:29:PRO:HD2	1:F:58:ASP:CG	2.19	0.63
1:E:141:LEU:HD22	1:E:371:LEU:N	2.13	0.62
1:C:277:ARG:HD2	1:D:311:TYR:CE2	2.34	0.62
1:F:203:ARG:HG3	1:F:235:LEU:HB3	1.81	0.62
1:A:34:LEU:HD22	2:A:440:HOH:O	1.98	0.62
1:C:307:ILE:HA	1:D:307:ILE:HD13	1.82	0.62
1:F:376:ASN:C	1:F:376:ASN:HD22	2.00	0.62
1:C:46:THR:N	2:C:16:HOH:O	2.32	0.62
1:D:30:MSE:HE2	1:D:94:ALA:N	2.14	0.62
1:D:157:ILE:HD11	1:D:338:GLU:HB3	1.81	0.62
1:F:29:PRO:HD2	1:F:58:ASP:OD2	2.00	0.62
1:F:232:ILE:HD12	1:F:237:ILE:HG13	1.81	0.62
1:B:67:THR:HG22	2:B:416:HOH:O	1.99	0.62
1:C:254:ARG:NH1	1:C:255:ASP:OD1	2.32	0.62
1:C:376:ASN:ND2	1:C:376:ASN:C	2.50	0.62
1:A:99:ARG:HG3	1:A:99:ARG:NH1	2.11	0.62
1:A:253:MSE:HE1	1:A:285:ILE:HG23	1.78	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLY:C	2:B:429:HOH:O	2.38	0.62
1:C:232:ILE:HD12	1:C:237:ILE:HG13	1.82	0.62
1:C:288:CYS:HB3	2:C:422:HOH:O	1.98	0.62
1:A:38:PHE:N	1:A:38:PHE:CD2	2.67	0.62
1:A:32:ALA:N	2:A:446:HOH:O	2.32	0.61
1:B:31:VAL:HG23	1:B:56:HIS:HB2	1.82	0.61
1:B:277:ARG:CZ	2:B:412:HOH:O	2.47	0.61
1:A:129:ILE:O	1:A:133:VAL:HG13	2.00	0.61
1:A:277:ARG:NH1	1:A:278:ASP:OD2	2.33	0.61
1:C:50:THR:HG22	1:C:347:PHE:CE2	2.31	0.61
1:B:101:TRP:CZ3	1:B:296:GLY:O	2.54	0.61
1:B:253:MSE:CA	1:B:256:VAL:HG12	2.28	0.61
1:E:30:MSE:SE	2:E:433:HOH:O	2.68	0.61
1:E:221:LYS:HE3	1:E:245:GLU:OE2	1.99	0.61
1:F:250:LYS:HG2	1:F:279:LEU:CD1	2.30	0.61
1:C:157:ILE:HG12	1:C:184:LYS:HE2	1.83	0.61
1:C:318:HIS:CE1	1:C:319:GLU:OE2	2.54	0.61
1:D:356:PRO:HG2	1:D:363:LEU:CD1	2.30	0.61
1:F:141:LEU:CD2	1:F:371:LEU:HD13	2.27	0.61
1:B:154:MSE:SE	2:B:425:HOH:O	2.68	0.61
1:B:253:MSE:CE	1:B:264:VAL:HG12	2.27	0.61
1:A:28:ILE:HG13	1:A:94:ALA:HB3	1.81	0.61
1:C:188:GLY:HA2	1:C:220:TYR:CZ	2.34	0.61
1:F:141:LEU:HG	1:F:145:TRP:CZ2	2.35	0.61
1:A:50:THR:N	1:A:74:MSE:HE1	2.15	0.60
1:C:315:MSE:HA	2:C:422:HOH:O	2.00	0.60
1:C:203:ARG:HG2	1:C:212:ILE:HD12	1.82	0.60
1:D:126:ASN:ND2	1:D:298:PRO:HD2	2.16	0.60
1:D:106:LYS:O	1:D:109:PHE:HB2	2.02	0.60
1:F:38:PHE:O	1:F:39:ARG:HG3	2.01	0.60
1:F:168:ILE:O	1:F:172:MSE:HG2	2.02	0.60
1:E:49:ALA:O	1:E:69:ASP:HA	2.01	0.60
1:E:89:LEU:HD23	1:E:100:LEU:HD22	1.84	0.60
1:F:191:SER:OG	1:F:194:GLU:HG3	2.01	0.60
1:A:203:ARG:HG3	1:A:235:LEU:HB3	1.82	0.60
1:E:171:GLU:HG2	1:E:175:TYR:CE2	2.35	0.60
1:B:254:ARG:NH1	1:C:258:TYR:OH	2.35	0.60
1:E:274:SER:O	1:E:277:ARG:HG3	2.01	0.60
1:A:268:GLN:HE21	1:A:289:ASN:HD21	1.50	0.60
1:B:376:ASN:C	1:B:376:ASN:HD22	2.05	0.60
1:D:232:ILE:HA	1:D:235:LEU:HD23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:ASP:OD1	1:E:247:HIS:HE1	1.85	0.60
1:B:155:ILE:HG23	1:B:336:ILE:HG21	1.83	0.59
1:E:28:ILE:N	2:E:11:HOH:O	2.35	0.59
1:E:254:ARG:HD3	1:E:282:THR:O	2.02	0.59
1:E:352:ILE:HG23	1:E:373:TRP:HB3	1.83	0.59
1:B:292:SER:HB3	1:B:317:HIS:NE2	2.16	0.59
1:D:61:ILE:HD12	1:D:135:LYS:HB3	1.84	0.59
1:E:347:PHE:HB3	1:E:351:MSE:HG3	1.84	0.59
1:C:307:ILE:HA	1:D:307:ILE:CD1	2.32	0.59
1:A:67:THR:HG23	2:A:8:HOH:O	2.01	0.59
1:B:253:MSE:HA	1:B:256:VAL:CG1	2.30	0.59
1:F:126:ASN:HD22	1:F:298:PRO:HD2	1.66	0.59
1:F:354:ASN:H	1:F:354:ASN:ND2	2.00	0.59
1:B:126:ASN:HD21	1:B:299:THR:H	1.49	0.59
1:C:129:ILE:O	1:C:133:VAL:HG12	2.03	0.59
1:E:322:GLN:HG2	1:E:323:VAL:HG23	1.83	0.59
1:A:28:ILE:N	2:A:442:HOH:O	2.35	0.59
1:A:99:ARG:HH11	1:A:99:ARG:CG	2.10	0.59
1:E:184:LYS:HE3	2:E:445:HOH:O	2.02	0.59
1:E:352:ILE:HG22	1:E:354:ASN:H	1.68	0.59
1:A:277:ARG:HG2	1:A:277:ARG:NH1	2.11	0.59
1:E:37:GLU:CD	1:E:37:GLU:N	2.56	0.59
1:E:141:LEU:HD11	2:E:431:HOH:O	2.03	0.59
1:C:253:MSE:CA	1:C:256:VAL:HG12	2.30	0.59
1:B:67:THR:HG23	1:B:293:SER:CB	2.31	0.59
1:B:348:TRP:NE1	2:B:425:HOH:O	2.32	0.59
1:C:311:TYR:CZ	1:D:277:ARG:HD2	2.37	0.59
1:C:377:TRP:O	1:C:381:ASP:HB2	2.03	0.59
1:C:381:ASP:HA	1:C:384:ARG:CD	2.33	0.59
1:F:354:ASN:HD22	1:F:354:ASN:N	1.95	0.59
1:B:31:VAL:CG2	1:B:56:HIS:HB2	2.33	0.58
1:D:28:ILE:O	1:D:28:ILE:HG13	2.03	0.58
1:E:163:GLU:OE1	1:E:167:SER:HA	2.02	0.58
1:C:34:LEU:CD2	1:C:54:ARG:HD3	2.32	0.58
1:C:38:PHE:CE1	1:C:380:ILE:HG23	2.38	0.58
1:A:30:MSE:HA	2:A:453:HOH:O	2.04	0.58
1:C:250:LYS:HG2	1:C:279:LEU:CD1	2.33	0.58
1:D:67:THR:HG23	1:D:293:SER:CB	2.22	0.58
1:A:376:ASN:ND2	1:A:378:ASP:HB2	2.15	0.58
1:C:356:PRO:HG2	1:C:363:LEU:HD21	1.86	0.58
1:E:188:GLY:HA2	1:E:220:TYR:CZ	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HG	1:A:145:TRP:CZ2	2.39	0.58
1:F:356:PRO:HB2	1:F:363:LEU:CD1	2.34	0.58
1:D:269:THR:O	1:D:269:THR:HG22	2.04	0.57
1:D:277:ARG:HH11	1:D:277:ARG:CG	2.14	0.57
1:A:30:MSE:SE	2:A:453:HOH:O	2.72	0.57
1:A:174:ASN:HD21	1:A:341:HIS:HE2	1.52	0.57
1:C:38:PHE:C	2:C:453:HOH:O	2.42	0.57
1:C:97:ILE:HD11	1:C:133:VAL:HG11	1.87	0.57
1:F:164:PRO:HG2	1:F:165:LEU:HD22	1.86	0.57
1:A:126:ASN:HD21	1:A:299:THR:H	1.51	0.57
1:A:352:ILE:HD12	1:A:354:ASN:N	2.20	0.57
1:B:199:ILE:HD13	1:B:214:ILE:HG21	1.86	0.57
1:D:95:MSE:HE2	1:D:133:VAL:HG12	1.86	0.57
1:F:30:MSE:SE	2:F:428:HOH:O	2.72	0.57
1:C:28:ILE:HG23	1:C:28:ILE:O	2.05	0.57
1:D:351:MSE:HE2	1:D:351:MSE:HA	1.87	0.57
1:D:253:MSE:HG3	1:D:284:ALA:HB1	1.85	0.57
1:E:33:PRO:HD3	1:E:90:ILE:HD11	1.87	0.57
1:E:277:ARG:NH2	1:F:310:SER:O	2.37	0.57
1:F:126:ASN:ND2	1:F:298:PRO:HD2	2.20	0.57
1:A:322:GLN:HG2	1:A:323:VAL:HG23	1.86	0.57
1:B:38:PHE:HE2	1:B:52:VAL:HG23	1.69	0.57
1:D:195:ASP:O	1:D:199:ILE:HG13	2.05	0.57
1:E:311:TYR:CE2	1:F:277:ARG:HD2	2.39	0.57
1:C:36:ARG:NH2	2:C:417:HOH:O	2.38	0.57
1:C:38:PHE:N	1:C:38:PHE:CD2	2.70	0.57
1:E:30:MSE:N	2:E:433:HOH:O	2.37	0.57
1:A:67:THR:HG21	1:A:124:ALA:HA	1.86	0.57
1:A:99:ARG:HG3	1:B:148:TYR:O	2.05	0.57
1:B:354:ASN:ND2	1:B:374:ASP:H	2.02	0.57
1:E:253:MSE:CE	1:E:264:VAL:HG12	2.34	0.57
1:A:31:VAL:HG22	1:A:56:HIS:C	2.25	0.56
1:C:130:TRP:HA	1:C:133:VAL:CG1	2.35	0.56
1:C:381:ASP:HA	1:C:384:ARG:HD3	1.87	0.56
1:F:354:ASN:HD21	1:F:374:ASP:H	1.53	0.56
1:C:38:PHE:HB2	1:C:383:TYR:O	2.05	0.56
1:E:156:ALA:HB2	1:E:180:LEU:HD13	1.86	0.56
1:E:250:LYS:HD3	1:E:279:LEU:HD13	1.87	0.56
1:E:371:LEU:CD1	1:E:373:TRP:CD1	2.84	0.56
1:F:164:PRO:HG2	1:F:165:LEU:CD2	2.35	0.56
1:D:371:LEU:HB3	1:D:373:TRP:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ILE:HB	1:C:340:PHE:CE1	2.41	0.56
1:C:93:ASP:OD1	1:C:95:MSE:HB2	2.06	0.56
1:D:254:ARG:NH1	1:D:255:ASP:OD1	2.38	0.56
1:F:356:PRO:HB2	1:F:363:LEU:HD12	1.85	0.56
1:E:174:ASN:HD21	1:E:341:HIS:HE2	1.53	0.56
1:E:356:PRO:HG2	1:E:363:LEU:HD11	1.88	0.56
1:F:38:PHE:CZ	1:F:380:ILE:HG12	2.40	0.56
1:A:301:TRP:CE3	1:A:327:LEU:HD22	2.40	0.56
1:F:57:THR:OG1	1:F:61:ILE:HG23	2.06	0.56
1:C:104:GLY:O	1:C:107:VAL:HG22	2.05	0.56
1:D:376:ASN:HD21	1:D:378:ASP:HB3	1.70	0.56
1:E:351:MSE:HE1	1:E:380:ILE:CD1	2.36	0.56
1:A:104:GLY:O	1:A:107:VAL:HG22	2.06	0.56
1:B:380:ILE:HG22	1:B:380:ILE:O	2.05	0.56
1:E:253:MSE:SE	2:E:450:HOH:O	2.73	0.56
1:C:253:MSE:O	1:C:256:VAL:HG12	2.05	0.56
1:C:67:THR:CG2	2:C:404:HOH:O	2.53	0.55
1:C:141:LEU:HD23	1:C:371:LEU:CD1	2.35	0.55
1:E:377:TRP:HA	1:E:380:ILE:HD13	1.86	0.55
1:A:171:GLU:HG2	1:A:175:TYR:CE2	2.41	0.55
1:B:29:PRO:HD2	1:B:58:ASP:CG	2.27	0.55
1:C:157:ILE:HB	1:C:340:PHE:CD1	2.42	0.55
1:E:95:MSE:HG3	1:F:139:MSE:HE1	1.87	0.55
1:F:61:ILE:CD1	1:F:135:LYS:HD2	2.37	0.55
1:A:258:TYR:OH	1:D:254:ARG:NH1	2.39	0.55
1:B:121:ALA:O	1:B:125:VAL:HG23	2.07	0.55
1:E:250:LYS:HD3	1:E:279:LEU:CD1	2.36	0.55
1:D:268:GLN:NE2	1:D:289:ASN:ND2	2.50	0.55
1:E:356:PRO:HG2	1:E:363:LEU:CD1	2.37	0.55
1:B:101:TRP:NE1	2:B:401:HOH:O	2.28	0.55
1:C:254:ARG:HH11	1:C:254:ARG:CG	2.18	0.55
1:E:38:PHE:N	1:E:38:PHE:CD2	2.74	0.55
1:A:156:ALA:HA	1:A:339:CYS:O	2.06	0.55
1:F:277:ARG:HG2	1:F:277:ARG:NH1	2.18	0.55
1:A:352:ILE:HG13	1:A:352:ILE:O	2.06	0.55
1:F:126:ASN:HD21	1:F:299:THR:H	1.54	0.55
1:A:249:ASP:OD1	1:A:250:LYS:N	2.39	0.55
1:B:33:PRO:CD	1:B:90:ILE:HD11	2.37	0.55
1:B:69:ASP:N	2:B:429:HOH:O	2.40	0.55
1:E:29:PRO:HA	1:E:92:GLN:O	2.07	0.55
1:E:220:TYR:HB2	1:E:243:PRO:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:ARG:HG3	1:E:344:ARG:NH1	2.20	0.55
1:E:376:ASN:HD22	1:E:378:ASP:H	1.53	0.55
1:C:203:ARG:NH2	1:C:210:PHE:O	2.35	0.55
1:D:37:GLU:HG3	1:D:75:PHE:HE1	1.72	0.55
1:D:376:ASN:ND2	1:D:378:ASP:HB3	2.22	0.55
1:E:149:ARG:NH1	1:E:151:GLU:O	2.40	0.55
1:E:253:MSE:SE	2:E:437:HOH:O	2.74	0.55
1:E:376:ASN:ND2	1:E:376:ASN:C	2.60	0.55
1:A:344:ARG:HH11	1:A:344:ARG:HG2	1.71	0.54
1:B:326:HIS:CD2	1:B:371:LEU:HD12	2.42	0.54
1:C:30:MSE:HG2	1:C:89:LEU:O	2.06	0.54
1:E:67:THR:HG23	1:E:293:SER:CB	2.38	0.54
1:E:41:SER:HB3	1:E:47:HIS:CE1	2.41	0.54
1:E:157:ILE:HB	1:E:340:PHE:CD1	2.43	0.54
1:F:222:PRO:O	1:F:226:VAL:HG23	2.08	0.54
1:A:116:ARG:HD2	1:A:294:TRP:CD1	2.42	0.54
1:B:340:PHE:HB2	1:B:345:ASP:HB3	1.89	0.54
1:B:358:LEU:HD13	1:B:363:LEU:HD13	1.89	0.54
1:C:33:PRO:HD3	1:C:90:ILE:HD11	1.88	0.54
1:C:253:MSE:CE	1:C:264:VAL:HG12	2.27	0.54
1:A:204:GLU:OE2	1:A:204:GLU:HA	2.06	0.54
1:C:160:TYR:CE1	1:C:186:LYS:NZ	2.71	0.54
1:F:253:MSE:HE1	1:F:266:ALA:HB2	1.88	0.54
1:B:365:LEU:N	1:B:365:LEU:HD22	2.22	0.54
1:E:95:MSE:CE	1:E:133:VAL:HB	2.37	0.54
1:E:141:LEU:HG	1:E:145:TRP:CH2	2.43	0.54
1:B:39:ARG:HD3	1:B:71:HIS:NE2	2.23	0.54
1:D:235:LEU:N	1:D:235:LEU:HD22	2.22	0.54
1:E:30:MSE:CE	1:E:89:LEU:HB3	2.25	0.54
1:B:168:ILE:O	1:B:172:MSE:HG2	2.08	0.54
1:D:277:ARG:HG2	1:D:277:ARG:NH1	2.17	0.54
1:C:89:LEU:CD1	1:C:125:VAL:HG11	2.34	0.54
1:F:33:PRO:CD	1:F:90:ILE:HD11	2.34	0.54
1:B:70:GLU:CD	1:B:70:GLU:H	2.12	0.53
1:B:184:LYS:CD	1:B:215:ASP:HB2	2.37	0.53
1:F:250:LYS:HG2	1:F:279:LEU:HD12	1.90	0.53
1:A:92:GLN:HB3	1:A:100:LEU:HD21	1.90	0.53
1:F:89:LEU:HD11	1:F:125:VAL:HG11	1.91	0.53
1:F:156:ALA:O	1:F:183:VAL:HG23	2.08	0.53
1:A:344:ARG:HG2	1:A:344:ARG:NH1	2.23	0.53
1:B:141:LEU:CD2	1:B:371:LEU:HD13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PRO:HD2	1:A:58:ASP:OD1	2.08	0.53
1:B:48:ARG:NH1	1:B:69:ASP:HB2	2.24	0.53
1:C:249:ASP:OD1	1:C:250:LYS:N	2.42	0.53
1:E:203:ARG:NH2	1:E:210:PHE:O	2.35	0.53
1:E:352:ILE:HD12	1:E:373:TRP:HB3	1.91	0.53
1:F:354:ASN:ND2	1:F:374:ASP:H	2.07	0.53
1:D:179:GLY:O	1:D:361:GLY:HA2	2.08	0.53
1:A:238:ARG:O	1:A:263:PRO:HG2	2.09	0.53
1:A:311:TYR:CZ	1:B:277:ARG:HD2	2.44	0.53
1:B:277:ARG:NH2	2:B:412:HOH:O	2.40	0.53
1:B:322:GLN:HG2	1:B:323:VAL:HG23	1.90	0.53
1:C:253:MSE:HE2	1:C:285:ILE:CG2	2.38	0.53
1:E:111:ILE:O	1:E:111:ILE:HG22	2.09	0.53
1:B:238:ARG:O	1:B:263:PRO:HG2	2.09	0.53
1:E:319:GLU:HA	1:E:338:GLU:HG3	1.90	0.53
1:B:38:PHE:CE2	1:B:52:VAL:HG23	2.43	0.52
1:F:238:ARG:O	1:F:263:PRO:HG2	2.09	0.52
1:A:76:ASP:O	1:A:80:ILE:HG13	2.10	0.52
1:A:172:MSE:N	1:A:172:MSE:HE2	2.23	0.52
1:B:195:ASP:O	1:B:199:ILE:HG13	2.08	0.52
1:C:310:SER:OG	1:D:277:ARG:HD3	2.10	0.52
1:C:33:PRO:CG	1:C:90:ILE:HD11	2.39	0.52
1:C:143:LYS:HD3	1:D:95:MSE:HG2	1.91	0.52
1:F:319:GLU:CD	1:F:340:PHE:HZ	2.12	0.52
1:B:48:ARG:HG3	1:B:346:PRO:HD2	1.91	0.52
1:C:277:ARG:HH11	1:C:277:ARG:CG	2.20	0.52
1:F:125:VAL:O	1:F:129:ILE:HG13	2.08	0.52
1:C:38:PHE:HE1	1:C:380:ILE:HG12	1.74	0.52
1:F:183:VAL:HG22	1:F:184:LYS:N	2.24	0.52
1:B:253:MSE:O	1:B:256:VAL:HG12	2.10	0.52
1:D:37:GLU:CD	1:D:37:GLU:N	2.60	0.52
1:E:252:SER:O	1:E:256:VAL:HG23	2.08	0.52
1:E:277:ARG:CA	1:E:280:MSE:HE3	2.36	0.52
1:B:29:PRO:HA	1:B:92:GLN:O	2.10	0.52
1:D:232:ILE:CA	1:D:235:LEU:HD23	2.40	0.52
1:F:76:ASP:HA	1:F:79:ARG:NH1	2.25	0.52
1:F:254:ARG:HH11	1:F:254:ARG:HG2	1.74	0.52
1:B:151:GLU:HA	1:B:363:LEU:O	2.09	0.52
1:C:95:MSE:HG2	1:D:139:MSE:HE1	1.93	0.52
1:F:54:ARG:HA	1:F:63:GLY:O	2.10	0.52
1:C:355:ARG:HH11	1:C:355:ARG:HG2	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:PRO:HG3	1:C:363:LEU:HD11	1.90	0.51
1:E:126:ASN:ND2	1:E:298:PRO:HD2	2.25	0.51
1:E:217:ASN:ND2	2:E:435:HOH:O	2.40	0.51
1:A:311:TYR:CE2	1:B:277:ARG:HD2	2.45	0.51
1:C:36:ARG:NH1	1:C:384:ARG:NH1	2.58	0.51
1:F:141:LEU:HD23	1:F:371:LEU:CD1	2.34	0.51
1:F:266:ALA:O	1:F:288:CYS:HA	2.10	0.51
1:A:49:ALA:O	1:A:69:ASP:HA	2.10	0.51
1:A:348:TRP:O	1:A:355:ARG:HD3	2.11	0.51
1:C:351:MSE:HE1	1:C:380:ILE:HD11	1.92	0.51
1:D:163:GLU:HB3	1:D:166:GLY:O	2.09	0.51
1:E:156:ALA:HA	1:E:339:CYS:O	2.11	0.51
1:A:126:ASN:HD22	1:A:298:PRO:HD2	1.75	0.51
1:B:257:ARG:HE	1:B:286:ASP:CG	2.13	0.51
1:C:269:THR:HG22	1:C:269:THR:O	2.10	0.51
1:D:351:MSE:HE3	1:D:379:TYR:CD2	2.44	0.51
1:B:254:ARG:HG2	1:B:254:ARG:NH1	2.20	0.51
1:A:37:GLU:CD	1:A:37:GLU:H	2.13	0.51
1:A:203:ARG:NH1	1:A:235:LEU:O	2.42	0.51
1:E:157:ILE:CD1	1:E:338:GLU:HB2	2.41	0.51
1:A:51:ILE:HG13	1:A:74:MSE:HE2	1.92	0.51
1:D:263:PRO:HA	1:D:286:ASP:OD2	2.11	0.51
1:E:351:MSE:HE3	1:E:379:TYR:CD2	2.38	0.51
1:B:31:VAL:HG22	1:B:56:HIS:C	2.31	0.51
1:E:38:PHE:HE1	1:E:351:MSE:SE	2.43	0.51
1:B:29:PRO:HD2	1:B:58:ASP:OD2	2.11	0.51
1:C:257:ARG:HE	1:C:286:ASP:CG	2.14	0.51
1:C:351:MSE:HE1	1:C:380:ILE:CG1	2.40	0.51
1:D:258:TYR:OH	1:E:254:ARG:NH1	2.44	0.51
1:E:351:MSE:HA	1:E:351:MSE:HE2	1.92	0.51
1:F:381:ASP:HA	2:F:433:HOH:O	2.10	0.51
1:E:50:THR:HG22	1:E:347:PHE:CE2	2.46	0.50
1:D:157:ILE:HG13	1:D:184:LYS:HE2	1.93	0.50
1:F:38:PHE:HZ	1:F:380:ILE:HG12	1.76	0.50
1:F:55:VAL:O	1:F:55:VAL:HG23	2.12	0.50
1:A:253:MSE:CE	1:A:285:ILE:HG22	2.40	0.50
1:C:371:LEU:HB3	1:C:373:TRP:CD1	2.45	0.50
1:E:38:PHE:HD2	1:E:38:PHE:N	2.07	0.50
1:E:151:GLU:HA	1:E:363:LEU:O	2.11	0.50
1:A:38:PHE:N	1:A:38:PHE:HD2	2.09	0.50
1:E:104:GLY:O	1:E:107:VAL:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:PHE:N	1:C:38:PHE:HD2	2.08	0.50
1:D:73:THR:O	1:D:76:ASP:HB2	2.11	0.50
1:E:48:ARG:HG3	1:E:347:PHE:CE2	2.46	0.50
1:F:171:GLU:HG2	1:F:172:MSE:HE2	1.94	0.50
1:F:355:ARG:HG2	2:F:416:HOH:O	2.12	0.50
1:A:253:MSE:HE2	1:A:285:ILE:HG23	1.91	0.50
1:C:285:ILE:HD12	1:C:288:CYS:HB2	1.93	0.50
1:D:357:LYS:NZ	1:D:357:LYS:HB3	2.26	0.50
1:E:95:MSE:CB	1:F:143:LYS:HD3	2.30	0.50
1:E:134:GLY:HA3	1:E:370:GLY:HA3	1.93	0.50
1:E:139:MSE:CE	1:F:95:MSE:HE2	2.42	0.50
1:F:38:PHE:CE1	1:F:52:VAL:HG23	2.47	0.50
1:C:34:LEU:HD21	1:C:36:ARG:HH21	1.75	0.50
1:E:307:ILE:HG12	1:F:307:ILE:HG12	1.94	0.50
1:F:156:ALA:HB2	1:F:180:LEU:CD1	2.41	0.50
1:A:162:GLY:C	1:A:163:GLU:HG2	2.32	0.50
1:B:54:ARG:HA	1:B:63:GLY:O	2.12	0.50
1:C:37:GLU:HB2	1:C:74:MSE:HE2	1.93	0.50
1:C:251:ARG:O	1:C:254:ARG:HB3	2.12	0.50
1:D:269:THR:O	1:D:269:THR:CG2	2.59	0.50
1:F:130:TRP:O	1:F:133:VAL:HG22	2.11	0.50
1:A:77:ILE:O	1:A:81:ILE:HG13	2.11	0.49
1:D:39:ARG:HE	1:D:71:HIS:CD2	2.30	0.49
1:D:89:LEU:O	1:D:92:GLN:HB2	2.12	0.49
1:F:116:ARG:HD2	1:F:294:TRP:CD1	2.47	0.49
1:D:38:PHE:HB2	1:D:50:THR:O	2.12	0.49
1:E:309:THR:N	2:E:443:HOH:O	2.43	0.49
1:E:371:LEU:CD1	1:E:372:GLY:N	2.72	0.49
1:A:46:THR:HG23	1:A:47:HIS:CD2	2.47	0.49
1:A:148:TYR:O	1:B:99:ARG:HD3	2.12	0.49
1:C:30:MSE:HB3	1:C:91:GLY:H	1.78	0.49
1:C:266:ALA:O	1:C:288:CYS:HA	2.12	0.49
1:D:356:PRO:HG2	1:D:363:LEU:CG	2.42	0.49
1:A:37:GLU:OE2	1:A:37:GLU:N	2.45	0.49
1:A:157:ILE:HB	1:A:340:PHE:CD1	2.47	0.49
1:C:184:LYS:HD3	1:C:215:ASP:HB2	1.94	0.49
1:B:249:ASP:O	1:B:253:MSE:HG2	2.13	0.49
1:C:188:GLY:HA2	1:C:220:TYR:CE1	2.47	0.49
1:D:140:PRO:HG2	1:D:143:LYS:HB3	1.95	0.49
1:B:151:GLU:HG3	1:B:363:LEU:O	2.12	0.49
1:C:67:THR:HG22	2:C:404:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ALA:HB3	1:A:87:PRO:HD3	1.95	0.49
1:C:55:VAL:HG23	1:C:128:ALA:HB1	1.94	0.49
1:C:356:PRO:HG2	1:C:363:LEU:CD2	2.43	0.49
1:E:253:MSE:CE	1:E:285:ILE:CG2	2.91	0.49
1:F:277:ARG:HH11	1:F:277:ARG:CG	2.20	0.48
1:D:34:LEU:HD21	1:D:54:ARG:HD3	1.94	0.48
1:E:254:ARG:HG2	1:E:254:ARG:NH1	2.28	0.48
1:F:303:ARG:O	1:F:307:ILE:HG13	2.13	0.48
1:A:38:PHE:HE2	1:A:50:THR:CG2	2.27	0.48
1:A:141:LEU:HD23	1:A:371:LEU:CD1	2.37	0.48
1:A:188:GLY:HA2	1:A:220:TYR:CZ	2.48	0.48
1:C:36:ARG:NH1	1:C:384:ARG:HH12	2.11	0.48
1:C:41:SER:HB3	1:C:47:HIS:CE1	2.49	0.48
1:C:277:ARG:HG2	1:C:277:ARG:NH1	2.22	0.48
1:D:156:ALA:HB2	1:D:180:LEU:HD13	1.95	0.48
1:D:250:LYS:HZ2	1:D:279:LEU:HD23	1.77	0.48
1:A:352:ILE:HG13	1:A:355:ARG:CG	2.44	0.48
1:B:184:LYS:HD3	1:B:215:ASP:CB	2.38	0.48
1:B:247:HIS:HE1	1:C:312:ASP:OD1	1.96	0.48
1:D:38:PHE:CZ	1:D:380:ILE:HG12	2.48	0.48
1:E:189:GLY:O	1:E:190:LEU:HD23	2.14	0.48
1:B:49:ALA:O	1:B:69:ASP:HA	2.13	0.48
1:B:119:LEU:HB3	1:B:295:SER:HA	1.95	0.48
1:E:168:ILE:HG23	1:E:172:MSE:HE3	1.96	0.48
1:E:318:HIS:ND1	1:E:319:GLU:HG2	2.28	0.48
1:A:30:MSE:HB2	1:A:89:LEU:O	2.13	0.48
1:B:68:GLY:O	1:B:69:ASP:CB	2.61	0.48
1:B:116:ARG:HD2	1:B:294:TRP:CD1	2.48	0.48
1:C:156:ALA:HB2	1:C:180:LEU:CD1	2.38	0.48
1:D:253:MSE:SE	2:D:458:HOH:O	2.81	0.48
1:E:126:ASN:ND2	1:E:299:THR:H	2.08	0.48
1:A:57:THR:HG22	2:A:453:HOH:O	2.14	0.48
1:D:30:MSE:CE	1:D:92:GLN:HB3	2.44	0.48
1:B:348:TRP:CD1	2:B:425:HOH:O	2.66	0.48
1:C:314:GLN:O	2:C:422:HOH:O	2.20	0.48
1:F:315:MSE:HG2	1:F:333:HIS:CD2	2.49	0.48
1:A:38:PHE:HZ	1:A:351:MSE:SE	2.47	0.48
1:C:218:GLN:HA	1:C:244:VAL:O	2.14	0.48
1:A:183:VAL:HG22	1:A:184:LYS:N	2.27	0.48
1:B:89:LEU:CD1	1:B:125:VAL:HG11	2.44	0.48
1:E:268:GLN:HE21	1:E:289:ASN:HD21	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLU:HB2	1:A:74:MSE:SE	2.64	0.47
1:A:73:THR:O	1:A:77:ILE:HG23	2.14	0.47
1:A:99:ARG:NH1	1:A:99:ARG:CG	2.72	0.47
1:A:151:GLU:HA	1:A:363:LEU:O	2.13	0.47
1:C:253:MSE:HE3	1:C:264:VAL:HG11	1.89	0.47
1:E:222:PRO:HG3	1:E:252:SER:HB3	1.96	0.47
1:C:29:PRO:HD2	1:C:58:ASP:OD1	2.14	0.47
1:C:30:MSE:HG2	1:C:90:ILE:N	2.28	0.47
1:E:48:ARG:HD2	1:E:69:ASP:OD1	2.13	0.47
1:E:92:GLN:HA	1:E:92:GLN:NE2	2.28	0.47
1:E:269:THR:HG22	1:E:269:THR:O	2.14	0.47
1:B:31:VAL:O	1:B:32:ALA:HB2	2.14	0.47
1:D:77:ILE:HD13	1:D:120:VAL:HG11	1.97	0.47
1:E:92:GLN:HA	1:E:92:GLN:HE21	1.79	0.47
1:E:272:SER:HB2	2:E:427:HOH:O	2.13	0.47
1:A:333:HIS:ND1	1:A:333:HIS:N	2.59	0.47
1:B:31:VAL:CG2	1:B:56:HIS:CB	2.92	0.47
1:C:77:ILE:HD13	1:C:120:VAL:HG11	1.96	0.47
1:D:203:ARG:HG3	1:D:235:LEU:HB3	1.97	0.47
1:A:74:MSE:SE	2:A:414:HOH:O	2.83	0.47
1:A:253:MSE:HE1	1:A:266:ALA:HB3	1.97	0.47
1:A:280:MSE:HG3	1:A:285:ILE:HD11	1.96	0.47
1:A:351:MSE:O	1:A:376:ASN:N	2.47	0.47
1:D:173:HIS:O	1:D:177:GLU:HG3	2.15	0.47
1:D:254:ARG:HG2	1:D:254:ARG:NH1	2.26	0.47
1:A:195:ASP:O	1:A:199:ILE:HG13	2.14	0.47
1:B:120:VAL:HG13	2:B:416:HOH:O	2.15	0.47
1:B:351:MSE:CE	1:B:380:ILE:HG12	2.41	0.47
1:B:376:ASN:HD22	1:B:378:ASP:H	1.61	0.47
1:C:38:PHE:HE2	1:C:50:THR:HG23	1.78	0.47
1:C:39:ARG:HD3	1:C:71:HIS:CD2	2.50	0.47
1:C:149:ARG:HD2	1:C:151:GLU:O	2.15	0.47
1:D:126:ASN:HD22	1:D:298:PRO:CD	2.27	0.47
1:D:232:ILE:HD12	1:D:237:ILE:HG13	1.97	0.47
1:A:28:ILE:HD12	1:A:57:THR:HG21	1.95	0.47
1:A:174:ASN:HD21	1:A:341:HIS:CD2	2.33	0.47
1:A:303:ARG:O	1:A:307:ILE:HG13	2.15	0.47
1:B:156:ALA:O	1:B:183:VAL:HA	2.15	0.47
1:B:377:TRP:CZ3	1:B:380:ILE:HD12	2.50	0.47
1:C:95:MSE:CE	1:C:133:VAL:HB	2.45	0.47
1:E:134:GLY:HA3	1:E:370:GLY:CA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ASN:HD22	1:B:354:ASN:N	1.96	0.47
1:C:126:ASN:ND2	1:C:299:THR:H	2.09	0.47
1:C:141:LEU:HD22	1:C:370:GLY:CA	2.43	0.47
1:C:274:SER:N	2:C:442:HOH:O	2.48	0.47
1:D:79:ARG:HG3	1:D:83:GLU:OE1	2.15	0.47
1:D:203:ARG:NH2	1:D:210:PHE:O	2.43	0.47
1:E:301:TRP:CZ2	1:E:315:MSE:HE3	2.50	0.47
1:E:318:HIS:HE1	2:E:448:HOH:O	1.98	0.47
1:D:37:GLU:N	1:D:37:GLU:OE2	2.48	0.47
1:E:34:LEU:CD2	2:E:441:HOH:O	2.63	0.47
1:E:342:PRO:HG3	1:E:349:TRP:CE2	2.50	0.47
1:A:39:ARG:NH2	2:A:422:HOH:O	2.48	0.46
1:C:253:MSE:HE1	1:C:285:ILE:HG22	1.95	0.46
1:F:195:ASP:O	1:F:199:ILE:HG13	2.15	0.46
1:F:344:ARG:HG3	1:F:344:ARG:HH11	1.80	0.46
1:A:30:MSE:CE	1:A:89:LEU:HD22	2.45	0.46
1:A:93:ASP:O	1:A:100:LEU:HD11	2.14	0.46
1:A:312:ASP:OD1	1:D:247:HIS:HE1	1.98	0.46
1:B:46:THR:HB	1:B:47:HIS:ND1	2.30	0.46
1:B:250:LYS:HD3	1:B:278:ASP:HB3	1.97	0.46
1:C:277:ARG:CD	1:D:311:TYR:CE2	2.97	0.46
1:D:36:ARG:CZ	2:D:460:HOH:O	2.63	0.46
1:D:86:ALA:N	1:D:87:PRO:CD	2.78	0.46
1:B:34:LEU:HD12	1:B:35:ALA:N	2.30	0.46
1:B:101:TRP:HH2	1:B:296:GLY:HA3	1.81	0.46
1:B:145:TRP:CE3	1:B:327:LEU:HD23	2.50	0.46
1:A:220:TYR:HB2	1:A:243:PRO:O	2.16	0.46
1:B:203:ARG:HG3	1:B:235:LEU:HB3	1.98	0.46
1:B:347:PHE:N	1:B:347:PHE:CD1	2.83	0.46
1:D:32:ALA:HA	1:D:33:PRO:HD3	1.76	0.46
1:E:249:ASP:OD1	1:E:250:LYS:N	2.48	0.46
1:F:354:ASN:ND2	1:F:354:ASN:N	2.62	0.46
1:D:149:ARG:O	1:D:329:ALA:HB1	2.16	0.46
1:F:68:GLY:O	1:F:69:ASP:C	2.54	0.46
1:C:221:LYS:HE2	1:C:245:GLU:OE2	2.15	0.46
1:A:143:LYS:HD3	1:B:95:MSE:HG2	1.97	0.46
1:C:39:ARG:CD	1:C:71:HIS:NE2	2.79	0.46
1:C:41:SER:HB3	1:C:47:HIS:ND1	2.31	0.46
1:E:253:MSE:HE2	1:E:285:ILE:CG2	2.45	0.46
1:A:156:ALA:HB2	1:A:180:LEU:CD1	2.36	0.46
1:B:226:VAL:HG22	1:B:256:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:PRO:CD	1:C:90:ILE:HD11	2.46	0.46
1:E:57:THR:O	1:E:59:ALA:O	2.34	0.46
1:F:38:PHE:CZ	1:F:380:ILE:HG23	2.50	0.46
1:A:38:PHE:HE1	1:A:380:ILE:HA	1.81	0.46
1:B:141:LEU:HD12	1:B:141:LEU:HA	1.67	0.46
1:C:182:GLY:HA2	1:C:210:PHE:CE1	2.50	0.46
1:E:66:TYR:HE2	1:E:352:ILE:HD11	1.81	0.46
1:E:172:MSE:SE	1:E:183:VAL:HG11	2.66	0.46
1:F:79:ARG:O	1:F:83:GLU:HG3	2.16	0.46
1:A:352:ILE:HD11	1:A:355:ARG:CA	2.46	0.46
1:E:32:ALA:HA	1:E:33:PRO:HD3	1.71	0.46
1:E:141:LEU:HD12	1:E:141:LEU:HA	1.78	0.46
1:A:46:THR:N	2:A:435:HOH:O	2.48	0.45
1:B:32:ALA:HA	1:B:33:PRO:HD3	1.72	0.45
1:E:370:GLY:O	1:E:371:LEU:CB	2.64	0.45
1:A:103:SER:O	1:A:106:LYS:HG2	2.17	0.45
1:B:376:ASN:HD21	1:B:378:ASP:CB	2.28	0.45
1:C:30:MSE:SE	1:C:55:VAL:HG13	2.66	0.45
1:C:36:ARG:HD3	1:C:384:ARG:NH1	2.31	0.45
1:B:67:THR:HG23	1:B:293:SER:HB3	1.99	0.45
1:E:78:ASP:HA	2:E:434:HOH:O	2.15	0.45
1:E:213:CYS:SG	1:E:238:ARG:HB3	2.56	0.45
1:B:70:GLU:O	1:B:70:GLU:HG2	2.16	0.45
1:C:253:MSE:HA	1:C:256:VAL:CG1	2.41	0.45
1:D:142:TRP:HB3	1:D:365:LEU:HD23	1.98	0.45
1:A:143:LYS:HD3	1:B:95:MSE:HB3	1.98	0.45
1:A:376:ASN:C	1:A:376:ASN:HD22	2.18	0.45
1:E:37:GLU:N	1:E:37:GLU:OE2	2.33	0.45
1:F:159:GLY:O	1:F:186:LYS:HB2	2.17	0.45
1:F:269:THR:HG22	1:F:269:THR:O	2.17	0.45
1:A:28:ILE:HD11	1:A:95:MSE:HE1	1.99	0.45
1:A:172:MSE:HG3	1:A:206:ALA:HB2	1.99	0.45
1:A:310:SER:OG	1:B:307:ILE:HD11	2.17	0.45
1:E:31:VAL:HG23	1:E:56:HIS:HB2	1.99	0.45
1:E:38:PHE:CE1	1:E:351:MSE:SE	3.20	0.45
1:C:180:LEU:HD23	1:C:358:LEU:CD1	2.47	0.45
1:F:109:PHE:N	1:F:109:PHE:CD1	2.84	0.45
1:F:318:HIS:C	1:F:319:GLU:HG2	2.37	0.45
1:B:266:ALA:O	1:B:288:CYS:HA	2.17	0.45
1:B:354:ASN:H	1:B:354:ASN:ND2	2.04	0.45
1:D:249:ASP:O	1:D:253:MSE:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:ILE:HG13	1:E:184:LYS:HE2	1.98	0.45
1:E:184:LYS:HD3	1:E:215:ASP:HB2	1.99	0.45
1:F:109:PHE:N	1:F:109:PHE:HD1	2.15	0.45
1:E:31:VAL:HG22	1:E:56:HIS:C	2.37	0.45
1:A:31:VAL:HG22	1:A:56:HIS:O	2.17	0.45
1:B:37:GLU:OE1	1:B:75:PHE:CE1	2.69	0.45
1:B:115:ARG:HD3	1:D:246:TRP:CE2	2.52	0.45
1:B:154:MSE:HE3	1:B:337:ALA:CB	2.47	0.45
1:C:28:ILE:CG2	1:C:94:ALA:HB3	2.42	0.45
1:C:30:MSE:CG	1:C:90:ILE:CA	2.90	0.45
1:C:340:PHE:HB3	1:C:344:ARG:HB3	1.99	0.45
1:E:301:TRP:CE2	1:E:315:MSE:HE3	2.51	0.45
1:F:126:ASN:HD22	1:F:298:PRO:CD	2.29	0.45
1:F:376:ASN:C	1:F:376:ASN:ND2	2.67	0.45
1:A:73:THR:HB	1:A:117:LEU:HD21	1.99	0.44
1:B:53:THR:O	1:B:64:GLU:HA	2.17	0.44
1:B:253:MSE:C	1:B:256:VAL:HG12	2.37	0.44
1:C:137:LEU:O	1:C:139:MSE:HG2	2.17	0.44
1:C:322:GLN:HG2	1:C:323:VAL:HG23	1.99	0.44
1:D:30:MSE:HE3	1:D:92:GLN:HB3	1.99	0.44
1:D:351:MSE:HE1	1:D:380:ILE:CG1	2.31	0.44
1:A:377:TRP:CE3	1:A:380:ILE:HD12	2.51	0.44
1:B:182:GLY:HA2	1:B:210:PHE:CE1	2.52	0.44
1:B:318:HIS:HA	1:B:338:GLU:OE1	2.16	0.44
1:B:368:ARG:HD2	2:B:445:HOH:O	2.17	0.44
1:C:153:PRO:HA	1:C:362:THR:HA	1.98	0.44
1:D:148:TYR:CD2	1:D:332:PRO:HA	2.52	0.44
1:E:34:LEU:HD23	2:E:441:HOH:O	2.18	0.44
1:E:129:ILE:O	1:E:132:ALA:HB3	2.17	0.44
1:F:89:LEU:CD1	1:F:125:VAL:HG11	2.47	0.44
1:F:203:ARG:NH2	1:F:210:PHE:O	2.43	0.44
1:B:38:PHE:N	1:B:38:PHE:CD2	2.85	0.44
1:B:268:GLN:NE2	1:B:318:HIS:CD2	2.85	0.44
1:B:381:ASP:HB2	2:B:436:HOH:O	2.16	0.44
1:C:347:PHE:N	1:C:347:PHE:HD1	2.16	0.44
1:D:253:MSE:HB3	2:D:458:HOH:O	2.18	0.44
1:D:348:TRP:CE2	1:D:355:ARG:HD2	2.53	0.44
1:F:155:ILE:HG22	1:F:182:GLY:N	2.32	0.44
1:A:182:GLY:HA2	1:A:210:PHE:CZ	2.52	0.44
1:A:307:ILE:HD11	1:B:310:SER:OG	2.16	0.44
1:D:171:GLU:HG2	1:D:175:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:ILE:HA	2:E:413:HOH:O	2.17	0.44
1:E:141:LEU:HD13	1:E:370:GLY:HA2	2.00	0.44
1:E:351:MSE:HE1	1:E:380:ILE:HD12	2.00	0.44
1:B:347:PHE:CA	1:B:351:MSE:HG3	2.47	0.44
1:C:253:MSE:HE1	1:C:266:ALA:CB	2.47	0.44
1:C:347:PHE:N	1:C:347:PHE:CD1	2.85	0.44
1:D:38:PHE:CZ	1:D:351:MSE:SE	3.20	0.44
1:E:152:LEU:O	1:E:152:LEU:HD12	2.18	0.44
1:E:155:ILE:HG23	1:E:336:ILE:HG21	1.98	0.44
1:F:253:MSE:HG3	1:F:264:VAL:HG11	2.00	0.44
1:A:352:ILE:HD11	1:A:354:ASN:C	2.38	0.44
1:B:181:ALA:HB2	1:B:361:GLY:O	2.18	0.44
1:D:182:GLY:HA2	1:D:210:PHE:CZ	2.52	0.44
1:D:183:VAL:HG22	1:D:184:LYS:N	2.32	0.44
1:E:54:ARG:HE	1:E:64:GLU:HG2	1.83	0.44
1:E:183:VAL:HG22	1:E:184:LYS:N	2.33	0.44
1:A:250:LYS:HG2	1:A:279:LEU:CD1	2.44	0.44
1:B:269:THR:O	1:B:269:THR:HG22	2.18	0.44
1:B:277:ARG:HG2	1:B:277:ARG:NH1	2.30	0.44
1:D:163:GLU:OE1	1:D:167:SER:HA	2.18	0.44
1:E:30:MSE:HE1	1:E:89:LEU:HD22	2.00	0.44
1:C:34:LEU:HD21	1:C:36:ARG:HE	1.81	0.44
1:A:38:PHE:CZ	1:A:351:MSE:SE	3.21	0.44
1:A:143:LYS:HA	1:A:147:GLY:CA	2.48	0.44
1:B:70:GLU:CD	1:B:70:GLU:N	2.70	0.44
1:B:346:PRO:HG2	1:B:347:PHE:CD1	2.53	0.44
1:B:376:ASN:C	1:B:376:ASN:ND2	2.71	0.44
1:C:67:THR:HG23	1:C:293:SER:HB3	2.00	0.44
1:C:153:PRO:HA	1:C:361:GLY:O	2.18	0.44
1:D:148:TYR:CG	1:D:332:PRO:HA	2.52	0.44
1:F:33:PRO:HA	1:F:54:ARG:O	2.18	0.44
1:F:49:ALA:HB1	1:F:74:MSE:HE1	1.99	0.44
1:F:322:GLN:N	1:F:322:GLN:OE1	2.51	0.44
1:F:344:ARG:HG3	1:F:344:ARG:NH1	2.33	0.44
1:B:28:ILE:HG12	1:B:28:ILE:O	2.17	0.43
1:B:86:ALA:HB3	1:B:87:PRO:HD3	1.99	0.43
1:B:172:MSE:SE	1:B:183:VAL:HG11	2.69	0.43
1:D:131:ASP:HB2	1:D:371:LEU:CD2	2.48	0.43
1:D:266:ALA:O	1:D:288:CYS:HA	2.18	0.43
1:E:182:GLY:HA2	1:E:210:PHE:CZ	2.54	0.43
1:E:249:ASP:O	1:E:253:MSE:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:ALA:HA	1:F:339:CYS:O	2.18	0.43
1:A:30:MSE:HE2	1:A:89:LEU:HD22	2.00	0.43
1:C:104:GLY:CA	2:C:411:HOH:O	2.57	0.43
1:C:247:HIS:HE1	1:F:312:ASP:OD1	2.00	0.43
1:C:347:PHE:O	1:C:351:MSE:HB2	2.18	0.43
1:D:172:MSE:SE	1:D:183:VAL:HG11	2.68	0.43
1:E:103:SER:O	1:E:106:LYS:HG2	2.18	0.43
1:C:246:TRP:CE2	1:E:115:ARG:HD3	2.53	0.43
1:F:253:MSE:CG	1:F:284:ALA:HB1	2.46	0.43
1:A:355:ARG:NH1	1:A:355:ARG:HB2	2.34	0.43
1:B:135:LYS:HA	1:B:369:PRO:HB3	2.01	0.43
1:E:141:LEU:CD1	2:E:431:HOH:O	2.63	0.43
1:E:280:MSE:HE1	1:E:307:ILE:CG2	2.48	0.43
1:E:308:ALA:C	2:E:443:HOH:O	2.56	0.43
1:F:56:HIS:CD2	2:F:418:HOH:O	2.71	0.43
1:A:54:ARG:HA	1:A:63:GLY:O	2.19	0.43
1:A:352:ILE:CG1	1:A:355:ARG:HG3	2.48	0.43
1:B:85:LEU:HD13	1:B:125:VAL:HG21	2.00	0.43
1:C:39:ARG:HD3	1:C:71:HIS:NE2	2.33	0.43
1:C:254:ARG:NH1	1:C:254:ARG:CG	2.80	0.43
1:D:30:MSE:HE1	1:D:100:LEU:HD11	1.99	0.43
1:B:36:ARG:NE	2:B:421:HOH:O	2.51	0.43
1:B:49:ALA:HB1	1:B:74:MSE:HE1	2.00	0.43
1:F:141:LEU:HD12	1:F:141:LEU:HA	1.89	0.43
1:F:163:GLU:HB3	1:F:166:GLY:O	2.19	0.43
1:C:221:LYS:HE2	1:C:245:GLU:CD	2.38	0.43
1:D:157:ILE:CD1	1:D:338:GLU:HB3	2.48	0.43
1:E:68:GLY:O	1:E:69:ASP:CB	2.67	0.43
1:C:254:ARG:O	1:C:257:ARG:HB3	2.19	0.43
1:D:356:PRO:HG2	1:D:363:LEU:HG	1.99	0.43
1:E:354:ASN:HD22	1:E:354:ASN:HA	1.60	0.43
1:F:220:TYR:HB2	1:F:243:PRO:O	2.17	0.43
1:B:36:ARG:NH1	1:B:377:TRP:CZ3	2.86	0.43
1:B:279:LEU:HD12	1:B:279:LEU:HA	1.91	0.43
1:B:368:ARG:HA	1:B:369:PRO:HD3	1.84	0.43
1:C:70:GLU:HG2	1:C:77:ILE:HD11	2.00	0.43
1:E:380:ILE:HD12	1:E:380:ILE:H	1.84	0.43
1:F:346:PRO:HG2	1:F:347:PHE:CD1	2.54	0.43
1:A:77:ILE:HG13	1:A:78:ASP:N	2.34	0.43
1:A:155:ILE:HG22	1:A:182:GLY:N	2.34	0.43
1:A:277:ARG:NH2	1:F:248:ASN:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:PHE:HA	1:B:351:MSE:HG3	2.00	0.43
1:B:377:TRP:C	1:B:379:TYR:H	2.22	0.43
1:C:254:ARG:HG2	1:C:254:ARG:NH1	2.20	0.43
1:F:64:GLU:OE1	1:F:375:LEU:HD12	2.19	0.43
1:F:163:GLU:HA	2:F:403:HOH:O	2.19	0.43
1:F:200:THR:O	1:F:204:GLU:HG3	2.19	0.43
1:A:377:TRP:CD2	1:A:380:ILE:HD12	2.54	0.42
1:B:246:TRP:CE2	1:D:115:ARG:HD3	2.54	0.42
1:C:143:LYS:HD3	1:D:95:MSE:HB3	2.00	0.42
1:D:188:GLY:HA2	1:D:220:TYR:CZ	2.54	0.42
1:F:49:ALA:HB1	1:F:74:MSE:CE	2.47	0.42
1:F:104:GLY:O	1:F:107:VAL:HG22	2.19	0.42
1:B:163:GLU:OE1	1:B:167:SER:HA	2.19	0.42
1:C:34:LEU:CD2	1:C:54:ARG:HH11	2.23	0.42
1:E:37:GLU:HA	1:E:51:ILE:HA	2.01	0.42
1:E:168:ILE:O	1:E:172:MSE:HE2	2.17	0.42
1:F:203:ARG:HG2	1:F:212:ILE:HD12	2.01	0.42
1:F:254:ARG:HG2	1:F:254:ARG:NH1	2.34	0.42
1:B:31:VAL:HG22	1:B:56:HIS:O	2.20	0.42
1:B:68:GLY:HA3	1:B:70:GLU:OE1	2.19	0.42
1:C:50:THR:CG2	1:C:347:PHE:CE2	3.02	0.42
1:D:51:ILE:O	1:D:66:TYR:HA	2.19	0.42
1:E:106:LYS:HE3	2:E:414:HOH:O	2.19	0.42
1:E:188:GLY:HA2	1:E:220:TYR:CE1	2.55	0.42
1:F:66:TYR:C	1:F:67:THR:CG2	2.87	0.42
1:A:141:LEU:HD22	1:A:370:GLY:C	2.40	0.42
1:B:156:ALA:O	1:B:183:VAL:HG23	2.20	0.42
1:C:79:ARG:O	1:C:83:GLU:HB2	2.19	0.42
1:C:95:MSE:HE3	1:C:95:MSE:HA	2.01	0.42
1:D:161:TYR:OH	1:D:187:VAL:HA	2.19	0.42
1:E:86:ALA:N	1:E:87:PRO:HD2	2.34	0.42
1:E:95:MSE:HE1	1:E:133:VAL:HB	2.01	0.42
1:E:95:MSE:HE3	1:E:133:VAL:HB	2.01	0.42
1:E:268:GLN:NE2	1:E:318:HIS:CD2	2.87	0.42
1:E:369:PRO:O	1:E:370:GLY:C	2.58	0.42
1:A:116:ARG:O	1:A:120:VAL:HG23	2.20	0.42
1:A:141:LEU:HG	1:A:145:TRP:CH2	2.55	0.42
1:A:203:ARG:NH2	1:A:210:PHE:O	2.48	0.42
1:A:352:ILE:HD12	1:A:352:ILE:C	2.40	0.42
1:B:67:THR:CG2	1:B:293:SER:HB3	2.49	0.42
1:B:351:MSE:HE1	1:B:380:ILE:CG1	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:ILE:O	1:C:384:ARG:HG2	2.18	0.42
1:D:203:ARG:HG2	1:D:212:ILE:HD12	2.01	0.42
1:D:235:LEU:HD22	1:D:235:LEU:H	1.84	0.42
1:B:38:PHE:N	1:B:38:PHE:HD2	2.17	0.42
1:B:156:ALA:HB2	1:B:180:LEU:CD1	2.35	0.42
1:B:183:VAL:HG22	1:B:184:LYS:N	2.35	0.42
1:D:245:GLU:HA	2:D:397:HOH:O	2.20	0.42
1:E:141:LEU:HD22	1:E:371:LEU:HB2	2.01	0.42
1:F:242:GLU:OE2	1:F:268:GLN:NE2	2.53	0.42
1:B:104:GLY:O	1:B:107:VAL:HG22	2.19	0.42
1:B:336:ILE:HG22	1:B:337:ALA:O	2.20	0.42
1:C:37:GLU:N	1:C:37:GLU:OE2	2.41	0.42
1:C:156:ALA:HA	1:C:339:CYS:O	2.20	0.42
1:E:39:ARG:NE	1:E:71:HIS:CD2	2.87	0.42
1:A:253:MSE:HE2	1:A:284:ALA:HB1	2.02	0.42
1:A:326:HIS:CE1	1:A:365:LEU:HD13	2.55	0.42
1:B:30:MSE:CB	1:B:90:ILE:HA	2.46	0.42
1:E:39:ARG:NH2	2:E:436:HOH:O	2.53	0.42
1:F:213:CYS:SG	1:F:238:ARG:HB3	2.60	0.42
1:F:320:GLU:C	1:F:322:GLN:OE1	2.58	0.42
1:F:335:THR:OG1	1:F:336:ILE:N	2.49	0.42
1:F:351:MSE:O	1:F:375:LEU:HA	2.19	0.42
1:A:106:LYS:HB3	1:A:106:LYS:HE2	1.82	0.42
1:B:250:LYS:HG3	1:B:279:LEU:CD1	2.50	0.42
1:C:95:MSE:HE2	1:C:133:VAL:HB	2.02	0.42
1:A:95:MSE:HG3	1:B:139:MSE:HE1	2.01	0.42
1:D:319:GLU:HB2	1:D:320:GLU:H	1.67	0.42
1:E:49:ALA:O	1:E:50:THR:HB	2.20	0.42
1:E:221:LYS:HE3	1:E:245:GLU:CD	2.40	0.42
1:E:287:VAL:HG22	1:E:314:GLN:HB2	2.02	0.42
1:B:141:LEU:HD13	1:B:370:GLY:HA2	2.01	0.41
1:D:95:MSE:CE	1:D:133:VAL:HG12	2.49	0.41
1:D:126:ASN:ND2	1:D:299:THR:H	2.14	0.41
1:E:54:ARG:HA	1:E:63:GLY:O	2.20	0.41
1:F:70:GLU:CD	1:F:70:GLU:N	2.71	0.41
1:F:86:ALA:N	1:F:87:PRO:CD	2.83	0.41
1:F:155:ILE:HG23	1:F:336:ILE:HG21	2.01	0.41
1:A:38:PHE:CE1	1:A:380:ILE:HA	2.55	0.41
1:A:182:GLY:HA3	1:A:211:ILE:O	2.20	0.41
1:B:48:ARG:HD2	1:B:48:ARG:HA	1.92	0.41
1:B:184:LYS:HD3	1:B:215:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:HIS:C	1:B:319:GLU:HG3	2.39	0.41
1:C:126:ASN:ND2	1:C:298:PRO:HD2	2.35	0.41
1:C:340:PHE:HB2	1:C:345:ASP:HB3	2.02	0.41
1:C:347:PHE:HZ	2:C:453:HOH:O	2.03	0.41
1:D:184:LYS:HD3	1:D:215:ASP:HB2	2.01	0.41
1:D:318:HIS:NE2	1:D:319:GLU:OE2	2.53	0.41
1:D:345:ASP:OD1	1:D:347:PHE:HB2	2.19	0.41
1:F:157:ILE:HD12	1:F:340:PHE:CE1	2.55	0.41
1:F:376:ASN:ND2	1:F:378:ASP:H	2.18	0.41
1:C:30:MSE:HE2	1:C:30:MSE:HB2	1.71	0.41
1:D:141:LEU:HD23	1:D:371:LEU:HD13	2.02	0.41
1:B:381:ASP:N	1:B:381:ASP:OD2	2.53	0.41
1:C:36:ARG:HH11	1:C:384:ARG:NH1	2.18	0.41
1:C:73:THR:HB	1:C:117:LEU:HD21	2.01	0.41
1:C:95:MSE:HE2	1:C:133:VAL:HG23	2.02	0.41
1:C:139:MSE:HE1	1:D:95:MSE:CG	2.50	0.41
1:D:253:MSE:CG	1:D:284:ALA:HB1	2.48	0.41
1:E:287:VAL:HA	1:E:314:GLN:O	2.18	0.41
1:E:315:MSE:HG2	1:E:333:HIS:CD2	2.56	0.41
1:C:80:ILE:O	1:C:84:GLU:HB2	2.20	0.41
1:C:253:MSE:C	1:C:256:VAL:HG12	2.41	0.41
1:C:376:ASN:HD21	1:C:378:ASP:HB2	1.84	0.41
1:F:130:TRP:HA	1:F:133:VAL:HG22	2.02	0.41
1:A:268:GLN:NE2	1:A:318:HIS:CD2	2.88	0.41
1:B:376:ASN:ND2	1:B:378:ASP:H	2.17	0.41
1:B:379:TYR:C	1:B:381:ASP:H	2.24	0.41
1:C:54:ARG:HA	1:C:63:GLY:O	2.20	0.41
1:E:89:LEU:O	1:E:92:GLN:HG2	2.20	0.41
1:F:218:GLN:HA	1:F:244:VAL:O	2.20	0.41
1:C:76:ASP:O	1:C:80:ILE:HG13	2.21	0.41
1:D:135:LYS:HA	1:D:369:PRO:HB3	2.03	0.41
1:F:38:PHE:CE1	1:F:52:VAL:CG2	3.03	0.41
1:F:131:ASP:O	1:F:135:LYS:HG3	2.20	0.41
1:A:126:ASN:ND2	1:A:298:PRO:HD2	2.35	0.41
1:A:376:ASN:O	1:A:380:ILE:HG13	2.21	0.41
1:C:32:ALA:HA	1:C:33:PRO:HD3	1.60	0.41
1:C:351:MSE:HA	1:C:351:MSE:HE3	2.02	0.41
1:D:141:LEU:HA	1:D:141:LEU:HD12	1.81	0.41
1:D:153:PRO:HA	1:D:362:THR:HA	2.01	0.41
1:D:331:GLN:HB3	1:D:333:HIS:CE1	2.56	0.41
1:E:35:ALA:HB1	1:E:78:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:TRP:O	2:E:431:HOH:O	2.21	0.41
1:E:310:SER:HB3	1:F:277:ARG:HE	1.86	0.41
1:A:50:THR:CA	1:A:74:MSE:HE1	2.51	0.41
1:B:138:LYS:HE2	1:B:138:LYS:HB3	1.85	0.41
1:B:365:LEU:N	1:B:365:LEU:CD2	2.84	0.41
1:C:86:ALA:N	1:C:87:PRO:CD	2.83	0.41
1:C:287:VAL:HA	1:C:314:GLN:O	2.20	0.41
1:D:254:ARG:HH11	1:D:254:ARG:CG	2.26	0.41
1:E:30:MSE:CE	1:E:89:LEU:HD22	2.50	0.41
1:F:174:ASN:O	1:F:178:LEU:HG	2.21	0.41
1:F:290:PHE:CZ	1:F:295:SER:CB	3.04	0.41
1:F:352:ILE:HG22	1:F:354:ASN:HD22	1.85	0.41
1:F:368:ARG:HB2	2:F:430:HOH:O	2.20	0.41
1:C:38:PHE:HD2	1:C:38:PHE:H	1.69	0.41
1:E:37:GLU:HB2	1:E:74:MSE:SE	2.71	0.41
1:E:130:TRP:O	1:E:133:VAL:HG22	2.20	0.41
1:F:92:GLN:HB3	1:F:100:LEU:HD21	2.03	0.41
1:B:376:ASN:HD21	1:B:378:ASP:HB3	1.86	0.40
1:C:30:MSE:HB3	1:C:91:GLY:N	2.35	0.40
1:C:37:GLU:HB3	1:C:51:ILE:HG12	2.04	0.40
1:F:143:LYS:HA	1:F:147:GLY:CA	2.51	0.40
1:A:51:ILE:HD12	1:A:77:ILE:HD11	2.03	0.40
1:A:141:LEU:CD1	1:A:144:LEU:HD23	2.51	0.40
1:A:228:LEU:O	1:A:232:ILE:HG12	2.21	0.40
1:B:253:MSE:CE	1:B:285:ILE:CG2	2.93	0.40
1:D:148:TYR:CD1	1:D:332:PRO:HB3	2.56	0.40
1:A:331:GLN:HB3	1:A:333:HIS:ND1	2.35	0.40
1:B:353:THR:OG1	1:B:374:ASP:HB3	2.21	0.40
1:C:126:ASN:HD22	1:C:298:PRO:HD2	1.86	0.40
1:C:168:ILE:O	1:C:172:MSE:HG2	2.22	0.40
1:D:33:PRO:CD	1:D:90:ILE:HD11	2.39	0.40
1:E:38:PHE:CE1	1:E:380:ILE:HG13	2.55	0.40
1:E:342:PRO:HG3	1:E:349:TRP:CD2	2.56	0.40
1:A:340:PHE:HB2	1:A:345:ASP:HB3	2.04	0.40
1:B:39:ARG:NE	1:B:71:HIS:CD2	2.89	0.40
1:B:95:MSE:HE2	1:B:133:VAL:HB	2.03	0.40
1:B:154:MSE:HE1	1:B:321:PRO:HB3	2.03	0.40
1:C:333:HIS:ND1	1:C:333:HIS:N	2.69	0.40
1:D:36:ARG:NH2	2:D:460:HOH:O	2.54	0.40
1:E:321:PRO:HA	1:E:324:SER:OG	2.20	0.40
1:F:56:HIS:HD1	1:F:62:ILE:HG12	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ARG:HA	1:A:369:PRO:HD3	1.93	0.40
1:C:28:ILE:CD1	1:C:57:THR:HG21	2.49	0.40
1:C:38:PHE:CE1	1:C:380:ILE:HA	2.56	0.40
1:C:279:LEU:HD12	1:C:279:LEU:HA	1.96	0.40
1:E:96:ALA:HB1	1:F:147:GLY:O	2.21	0.40
1:F:277:ARG:NH1	1:F:278:ASP:OD2	2.46	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	345/379 (91%)	326 (94%)	16 (5%)	3 (1%)	17	31
1	B	347/379 (92%)	323 (93%)	22 (6%)	2 (1%)	25	43
1	C	351/379 (93%)	332 (95%)	17 (5%)	2 (1%)	25	43
1	D	347/379 (92%)	325 (94%)	18 (5%)	4 (1%)	13	24
1	E	346/379 (91%)	315 (91%)	26 (8%)	5 (1%)	11	20
1	F	347/379 (92%)	327 (94%)	18 (5%)	2 (1%)	25	43
All	All	2083/2274 (92%)	1948 (94%)	117 (6%)	18 (1%)	17	31

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	PRO
1	B	69	ASP
1	D	61	ILE
1	E	69	ASP
1	C	33	PRO
1	D	68	GLY

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Mol	Chain	Res	Type
1	E	33	PRO
1	E	370	GLY
1	F	69	ASP
1	E	372	GLY
1	F	33	PRO
1	A	319	GLU
1	C	187	VAL
1	D	33	PRO
1	A	187	VAL
1	B	33	PRO
1	D	187	VAL
1	E	187	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	280/297 (94%)	255 (91%)	25 (9%)	9	19
1	B	282/297 (95%)	259 (92%)	23 (8%)	11	22
1	C	286/297 (96%)	263 (92%)	23 (8%)	12	23
1	D	282/297 (95%)	265 (94%)	17 (6%)	19	37
1	E	281/297 (95%)	265 (94%)	16 (6%)	20	39
1	F	282/297 (95%)	262 (93%)	20 (7%)	14	28
All	All	1693/1782 (95%)	1569 (93%)	124 (7%)	14	27

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MSE
1	A	38	PHE
1	A	46	THR
1	A	77	ILE
1	A	95	MSE
1	A	99	ARG

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Mol	Chain	Res	Type
1	A	133	VAL
1	A	138	LYS
1	A	141	LEU
1	A	152	LEU
1	A	163	GLU
1	A	172	MSE
1	A	176	GLN
1	A	203	ARG
1	A	221	LYS
1	A	240	PHE
1	A	262	VAL
1	A	279	LEU
1	A	294	TRP
1	A	333	HIS
1	A	343	ASP
1	A	352	ILE
1	A	366	SER
1	A	371	LEU
1	A	376	ASN
1	B	30	MSE
1	B	34	LEU
1	B	38	PHE
1	B	46	THR
1	B	48	ARG
1	B	70	GLU
1	B	76	ASP
1	B	95	MSE
1	B	125	VAL
1	B	141	LEU
1	B	203	ARG
1	B	240	PHE
1	B	262	VAL
1	B	279	LEU
1	B	292	SER
1	B	333	HIS
1	B	351	MSE
1	B	354	ASN
1	B	358	LEU
1	B	371	LEU
1	B	374	ASP
1	B	376	ASN
1	B	378	ASP

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Mol	Chain	Res	Type
1	C	37	GLU
1	C	38	PHE
1	C	48	ARG
1	C	70	GLU
1	C	95	MSE
1	C	103	SER
1	C	111	ILE
1	C	133	VAL
1	C	141	LEU
1	C	184	LYS
1	C	203	ARG
1	C	221	LYS
1	C	240	PHE
1	C	268	GLN
1	C	279	LEU
1	C	351	MSE
1	C	360	ASN
1	C	363	LEU
1	C	364	THR
1	C	371	LEU
1	C	376	ASN
1	C	381	ASP
1	C	384	ARG
1	D	34	LEU
1	D	37	GLU
1	D	38	PHE
1	D	72	GLU
1	D	92	GLN
1	D	95	MSE
1	D	106	LYS
1	D	141	LEU
1	D	152	LEU
1	D	184	LYS
1	D	203	ARG
1	D	240	PHE
1	D	262	VAL
1	D	279	LEU
1	D	360	ASN
1	D	365	LEU
1	D	376	ASN
1	E	29	PRO
1	E	30	MSE

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Mol	Chain	Res	Type
1	E	70	GLU
1	E	90	ILE
1	E	95	MSE
1	E	141	LEU
1	E	203	ARG
1	E	221	LYS
1	E	240	PHE
1	E	277	ARG
1	E	351	MSE
1	E	354	ASN
1	E	371	LEU
1	E	376	ASN
1	E	378	ASP
1	E	381	ASP
1	F	34	LEU
1	F	36	ARG
1	F	48	ARG
1	F	61	ILE
1	F	70	GLU
1	F	83	GLU
1	F	141	LEU
1	F	152	LEU
1	F	176	GLN
1	F	203	ARG
1	F	240	PHE
1	F	254	ARG
1	F	262	VAL
1	F	354	ASN
1	F	360	ASN
1	F	365	LEU
1	F	371	LEU
1	F	376	ASN
1	F	378	ASP
1	F	381	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	174	ASN
1	A	217	ASN
1	A	247	HIS

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Mol	Chain	Res	Type
1	A	268	GLN
1	A	359	ASN
1	A	360	ASN
1	A	376	ASN
1	B	42	HIS
1	B	56	HIS
1	B	92	GLN
1	B	126	ASN
1	B	247	HIS
1	B	268	GLN
1	B	318	HIS
1	B	354	ASN
1	B	376	ASN
1	C	42	HIS
1	C	47	HIS
1	C	126	ASN
1	C	174	ASN
1	C	247	HIS
1	C	268	GLN
1	C	318	HIS
1	C	359	ASN
1	C	360	ASN
1	C	376	ASN
1	C	382	GLN
1	D	42	HIS
1	D	126	ASN
1	D	247	HIS
1	D	268	GLN
1	D	350	ASN
1	D	359	ASN
1	D	360	ASN
1	D	376	ASN
1	E	47	HIS
1	E	92	GLN
1	E	126	ASN
1	E	174	ASN
1	E	247	HIS
1	E	268	GLN
1	E	318	HIS
1	E	354	ASN
1	E	376	ASN
1	F	47	HIS

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Mol	Chain	Res	Type
1	F	71	HIS
1	F	126	ASN
1	F	247	HIS
1	F	268	GLN
1	F	354	ASN
1	F	359	ASN
1	F	376	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	339/379 (89%)	-0.27	0 100 100	10, 22, 37, 49	0
1	B	341/379 (89%)	-0.26	4 (1%) 79 80	10, 22, 37, 52	0
1	C	345/379 (91%)	-0.23	1 (0%) 94 94	10, 23, 38, 52	0
1	D	341/379 (89%)	-0.21	3 (0%) 84 86	10, 21, 36, 57	0
1	E	340/379 (89%)	0.04	4 (1%) 79 80	12, 27, 44, 61	0
1	F	341/379 (89%)	-0.06	3 (0%) 84 86	12, 26, 43, 57	0
All	All	2047/2274 (90%)	-0.17	15 (0%) 87 89	10, 23, 40, 61	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	68	GLY	3.3
1	B	42	HIS	3.0
1	F	42	HIS	2.9
1	B	46	THR	2.8
1	F	41	SER	2.5
1	E	177	GLU	2.4
1	B	378	ASP	2.4
1	D	33	PRO	2.2
1	F	47	HIS	2.1
1	D	209	ASP	2.1
1	B	68	GLY	2.1
1	E	36	ARG	2.1
1	D	38	PHE	2.1
1	E	168	ILE	2.0
1	C	38	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.