



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:22 PM GMT

PDB ID : 3R3J  
Title : Kinetic and structural characterization of Plasmodium falciparum glutamate dehydrogenase 2  
Authors : Zocher, K.; Fritz-Wolf, K.; Kehr, S.; Rahlfs, S.; Becker, K.  
Deposited on : 2011-03-16  
Resolution : 3.10 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

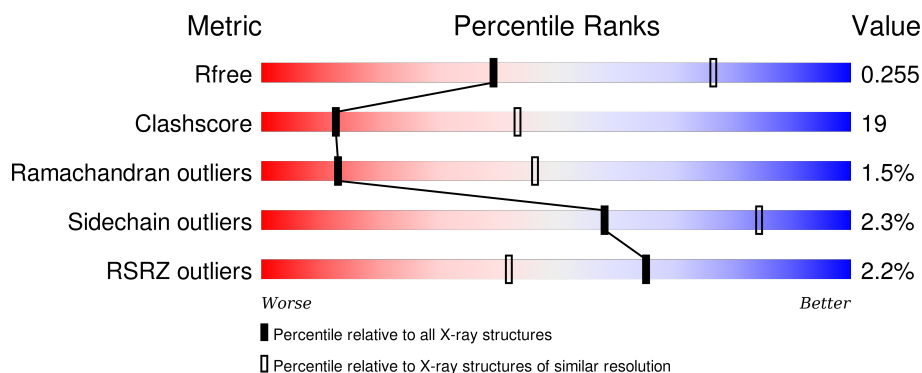
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	456	<div> <div>67%</div> <div>31%</div> <div>•</div> </div>
1	B	456	<div> <div>65%</div> <div>32%</div> <div>•</div> </div>
1	C	456	<div> <div>65%</div> <div>33%</div> <div>•</div> </div>
1	D	456	<div> <div>65%</div> <div>34%</div> <div>•</div> </div>
1	E	456	<div> <div>63%</div> <div>34%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	456	 A horizontal bar chart showing the quality of the chain. The bar is divided into two segments: a green segment on the left representing 65% and a yellow segment on the right representing 33%. A small orange square is at the far right end of the bar, and a small black dot is at the end of the yellow segment.

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 21631 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3602	2290	615	678	19			
1	B	456	Total	C	N	O	S	0	0	0
			3602	2290	615	678	19			
1	C	456	Total	C	N	O	S	0	0	0
			3602	2290	615	678	19			
1	D	456	Total	C	N	O	S	0	0	0
			3602	2290	615	678	19			
1	E	456	Total	C	N	O	S	0	0	0
			3602	2290	615	678	19			
1	F	456	Total	C	N	O	S	0	0	0
			3602	2290	615	678	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	ALA	THR	ENGINEERED MUTATION	UNP Q8ILF7
B	161	ALA	THR	ENGINEERED MUTATION	UNP Q8ILF7
C	161	ALA	THR	ENGINEERED MUTATION	UNP Q8ILF7
D	161	ALA	THR	ENGINEERED MUTATION	UNP Q8ILF7
E	161	ALA	THR	ENGINEERED MUTATION	UNP Q8ILF7
F	161	ALA	THR	ENGINEERED MUTATION	UNP Q8ILF7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	3	Total	O	0	0
			3	3		
2	C	2	Total	O	0	0
			2	2		

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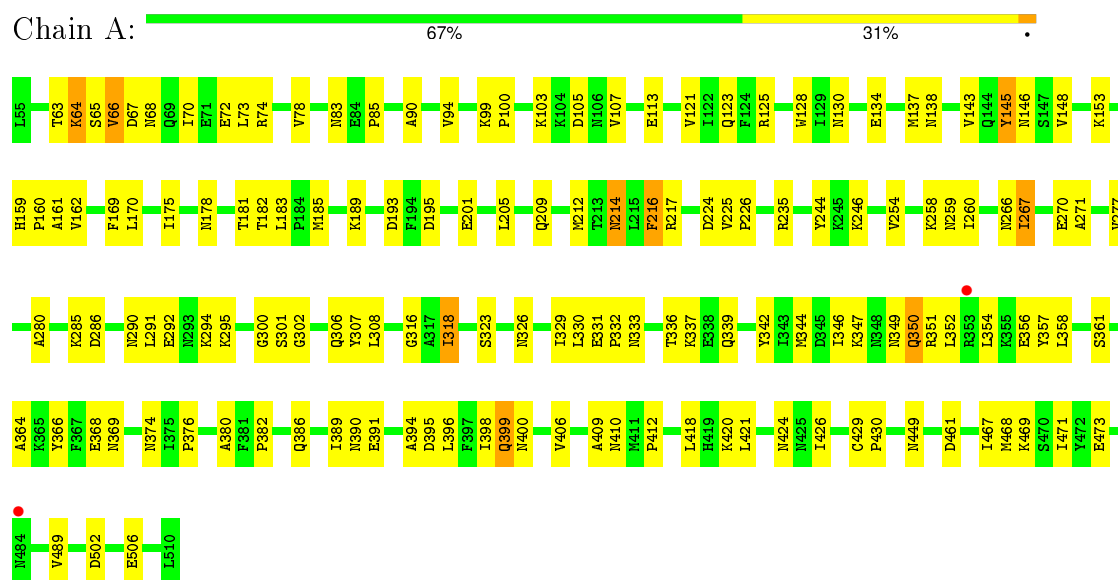
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	O	0	0
			2	2		
2	E	4	Total	O	0	0
			4	4		
2	F	5	Total	O	0	0
			5	5		

### 3 Residue-property plots [i](#)

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

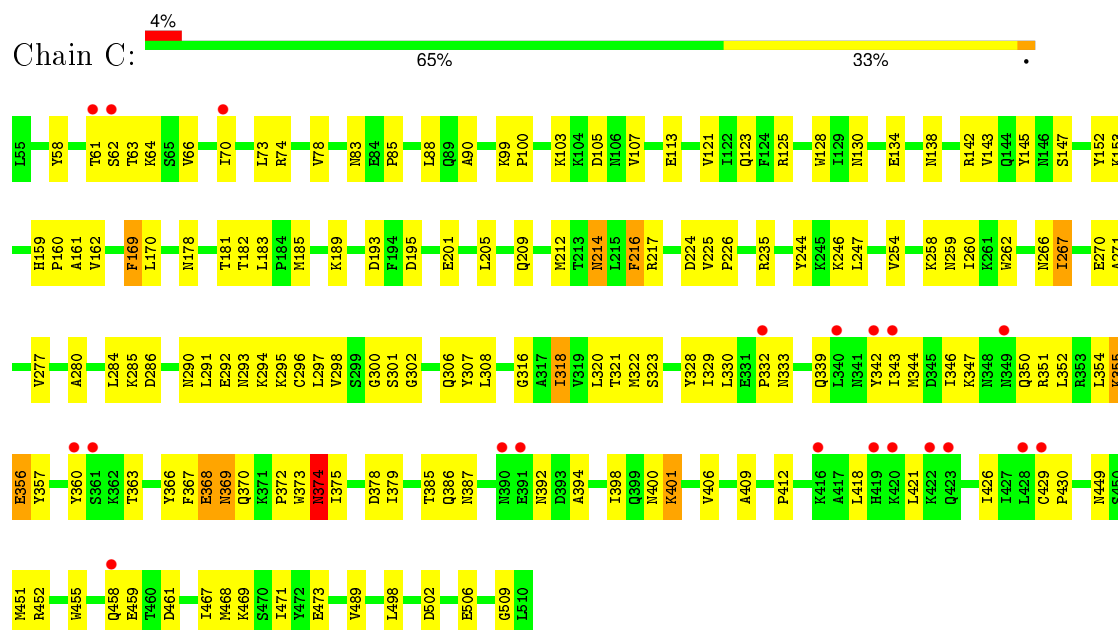
#### • Molecule 1: Glutamate dehydrogenase



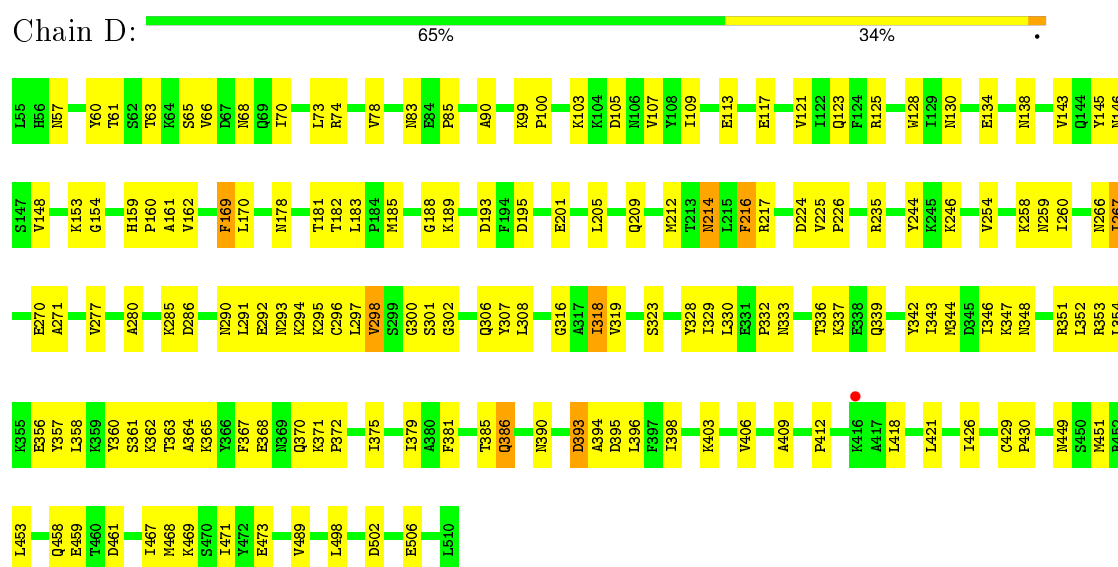
#### • Molecule 1: Glutamate dehydrogenase



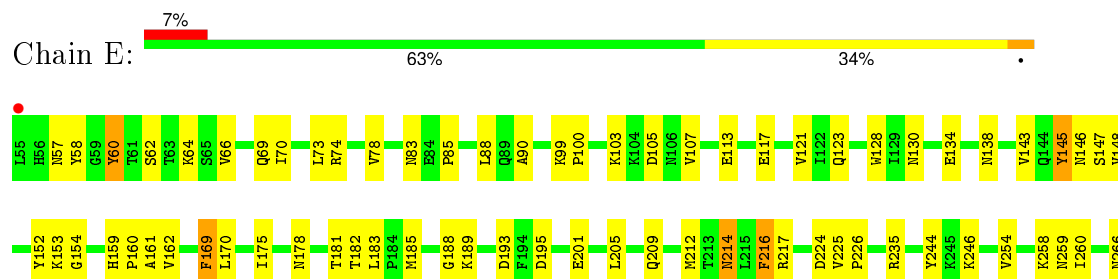
- Molecule 1: Glutamate dehydrogenase

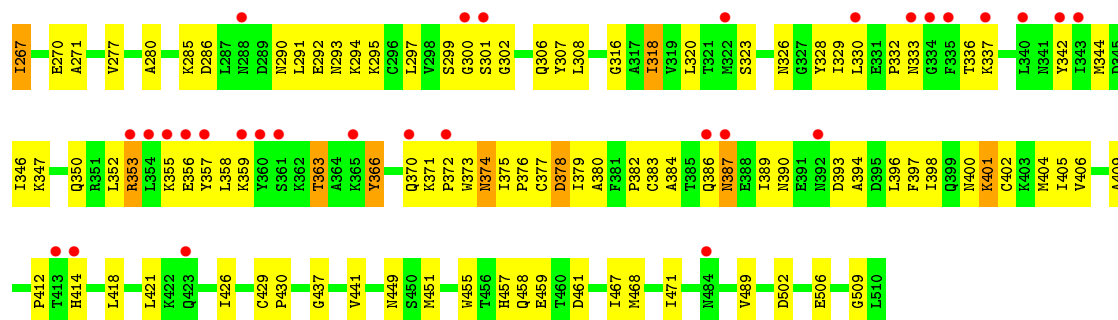


- Molecule 1: Glutamate dehydrogenase



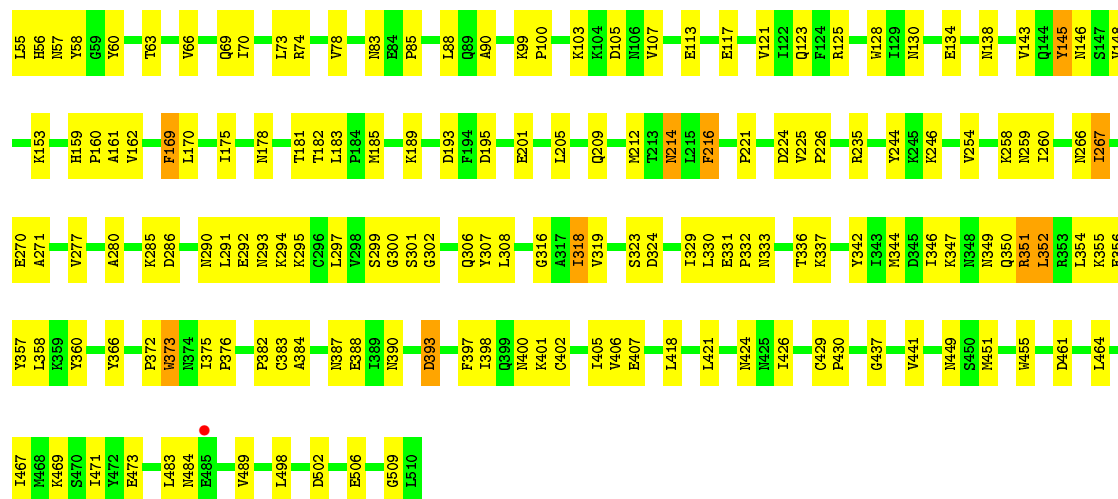
- Molecule 1: Glutamate dehydrogenase





• Molecule 1: Glutamate dehydrogenase

Chain F: 65% 33% •





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.78Å 140.01Å 180.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 3.10 47.55 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.99-3.10) 99.6 (47.55-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 3.12Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.231 , 0.258 0.233 , 0.255	Depositor DCC
$R_{free}$ test set	3200 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.9	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.4	EDS
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 675767 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	21631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.40	0/3672	0.58	0/4944
1	B	0.43	0/3672	0.59	0/4944
1	C	0.42	0/3672	0.58	0/4944
1	D	0.42	0/3672	0.58	0/4944
1	E	0.43	0/3672	0.59	0/4944
1	F	0.41	0/3672	0.59	0/4944
All	All	0.42	0/22032	0.59	0/29664

There are no bond length outliers.

There are no bond angle outliers.

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	3602	0	3597	128	0
1	B	3602	0	3597	146	0
1	C	3602	0	3597	149	0
1	D	3602	0	3597	145	0
1	E	3602	0	3597	156	0
1	F	3602	0	3597	150	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	4	0	0	2	0
2	F	5	0	0	0	0
All	All	21631	0	21582	836	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 19.

All (836) 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:F:292:GLU:HA	1:F:316:GLY:HA3	1.38	1.05
1:D:300:GLY:H	1:D:323:SER:HB3	1.19	1.04
1:E:292:GLU:HA	1:E:316:GLY:HA3	1.37	1.03
1:B:292:GLU:HA	1:B:316:GLY:HA3	1.38	1.03
1:A:292:GLU:HA	1:A:316:GLY:HA3	1.37	1.02
1:C:292:GLU:HA	1:C:316:GLY:HA3	1.40	1.02
1:D:292:GLU:HA	1:D:316:GLY:HA3	1.38	1.01
1:C:300:GLY:H	1:C:323:SER:HB3	1.23	0.99
1:E:300:GLY:H	1:E:323:SER:HB3	1.35	0.90
1:D:329:ILE:CD1	1:D:354:LEU:HG	2.02	0.89
1:D:329:ILE:HD12	1:D:354:LEU:HG	1.53	0.89
1:C:401:LYS:NZ	1:C:401:LYS:HA	1.88	0.88
1:B:58:TYR:OH	1:B:509:GLY:HA3	1.73	0.88
1:C:181:THR:HG22	1:C:183:LEU:H	1.41	0.85
1:B:430:PRO:HG3	1:B:489:VAL:HA	1.58	0.84
1:E:430:PRO:HG3	1:E:489:VAL:HA	1.58	0.84
1:E:277:VAL:HG23	1:E:308:LEU:HD12	1.59	0.84
1:A:181:THR:HG22	1:A:183:LEU:H	1.43	0.84
1:D:181:THR:HG22	1:D:183:LEU:H	1.41	0.83
1:B:181:THR:HG22	1:B:183:LEU:H	1.44	0.83
1:D:430:PRO:HG3	1:D:489:VAL:HA	1.60	0.82
1:A:430:PRO:HG3	1:A:489:VAL:HA	1.59	0.82
1:C:290:ASN:HD21	1:C:292:GLU:HB2	1.44	0.82
1:C:244:TYR:CZ	1:C:254:VAL:HG11	2.15	0.82
1:F:181:THR:O	1:F:182:THR:HB	1.78	0.82
1:F:277:VAL:HG23	1:F:308:LEU:HD12	1.62	0.82
1:F:181:THR:HG22	1:F:183:LEU:H	1.44	0.82
1:F:430:PRO:HG3	1:F:489:VAL:HA	1.62	0.82
1:C:430:PRO:HG3	1:C:489:VAL:HA	1.60	0.82
1:D:181:THR:O	1:D:182:THR:HB	1.80	0.81
1:B:181:THR:O	1:B:182:THR:HB	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:PRO:HA	1:B:400:ASN:HB3	1.61	0.81
1:A:290:ASN:HD21	1:A:292:GLU:HB2	1.44	0.81
1:A:181:THR:O	1:A:182:THR:HB	1.80	0.81
1:E:181:THR:O	1:E:182:THR:HB	1.81	0.80
1:D:290:ASN:HD21	1:D:292:GLU:HB2	1.46	0.80
1:C:201:GLU:OE2	1:C:235:ARG:HD2	1.81	0.80
1:B:290:ASN:HD21	1:B:292:GLU:HB2	1.47	0.79
1:C:181:THR:O	1:C:182:THR:HB	1.80	0.79
1:E:181:THR:HG22	1:E:183:LEU:H	1.45	0.79
1:C:277:VAL:HG23	1:C:308:LEU:HD12	1.64	0.79
1:E:290:ASN:HD21	1:E:292:GLU:HB2	1.46	0.79
1:F:244:TYR:CZ	1:F:254:VAL:HG11	2.17	0.79
1:D:244:TYR:CZ	1:D:254:VAL:HG11	2.18	0.79
1:F:201:GLU:OE2	1:F:235:ARG:HD2	1.82	0.79
1:B:244:TYR:CZ	1:B:254:VAL:HG11	2.18	0.79
1:E:244:TYR:CZ	1:E:254:VAL:HG11	2.18	0.79
1:E:201:GLU:OE2	1:E:235:ARG:HD2	1.83	0.78
1:D:277:VAL:HG23	1:D:308:LEU:HD12	1.64	0.78
1:A:244:TYR:CZ	1:A:254:VAL:HG11	2.19	0.78
1:A:300:GLY:H	1:A:323:SER:HB3	1.47	0.78
1:A:277:VAL:HG23	1:A:308:LEU:HD12	1.65	0.78
1:D:201:GLU:OE2	1:D:235:ARG:HD2	1.85	0.77
1:F:300:GLY:H	1:F:323:SER:HB3	1.50	0.77
1:C:342:TYR:CD1	1:C:360:TYR:HB3	2.20	0.77
1:F:290:ASN:HD21	1:F:292:GLU:HB2	1.48	0.77
1:C:350:GLN:HB3	1:C:352:LEU:HG	1.66	0.77
1:F:350:GLN:HB3	1:F:352:LEU:HD11	1.67	0.77
1:B:277:VAL:HG23	1:B:308:LEU:HD12	1.65	0.77
1:C:401:LYS:HA	1:C:401:LYS:HZ2	1.48	0.76
1:F:351:ARG:HH11	1:F:351:ARG:HB3	1.51	0.76
1:B:201:GLU:OE2	1:B:235:ARG:HD2	1.85	0.76
1:A:201:GLU:OE2	1:A:235:ARG:HD2	1.85	0.76
1:C:297:LEU:HD13	1:C:372:PRO:O	1.87	0.75
1:E:297:LEU:HG	1:E:377:CYS:HB2	1.67	0.75
1:F:160:PRO:HG3	1:F:195:ASP:HB2	1.68	0.75
1:B:123:GLN:HB3	1:C:121:VAL:HG13	1.67	0.74
1:D:300:GLY:N	1:D:323:SER:HB3	2.00	0.74
1:D:134:GLU:HG2	1:F:57:ASN:HD21	1.52	0.74
1:B:121:VAL:HG13	1:C:123:GLN:HB3	1.69	0.74
1:A:361:SER:HB3	1:A:364:ALA:HB2	1.68	0.73
1:E:430:PRO:CG	1:E:489:VAL:HA	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PRO:HG3	1:C:195:ASP:HB2	1.70	0.73
1:F:351:ARG:NH1	1:F:351:ARG:HB3	2.03	0.73
1:A:160:PRO:HG3	1:A:195:ASP:HB2	1.69	0.73
1:C:430:PRO:CG	1:C:489:VAL:HA	2.19	0.72
1:F:300:GLY:N	1:F:323:SER:HB3	2.05	0.72
1:B:214:ASN:N	1:B:214:ASN:HD22	1.88	0.72
1:D:297:LEU:HD13	1:D:372:PRO:O	1.88	0.71
1:F:329:ILE:HD13	1:F:357:TYR:HB3	1.73	0.71
1:B:160:PRO:HG3	1:B:195:ASP:HB2	1.73	0.70
1:A:430:PRO:CG	1:A:489:VAL:HA	2.21	0.70
1:E:292:GLU:HA	1:E:316:GLY:CA	2.20	0.70
1:D:430:PRO:CG	1:D:489:VAL:HA	2.20	0.70
1:B:430:PRO:CG	1:B:489:VAL:HA	2.20	0.70
1:C:394:ALA:O	1:C:398:ILE:HG13	1.90	0.70
1:C:214:ASN:N	1:C:214:ASN:HD22	1.89	0.70
1:B:292:GLU:HA	1:B:316:GLY:CA	2.20	0.70
1:B:329:ILE:HD13	1:B:357:TYR:CD2	2.26	0.69
1:F:214:ASN:N	1:F:214:ASN:HD22	1.89	0.69
1:E:214:ASN:N	1:E:214:ASN:HD22	1.90	0.69
1:E:160:PRO:HG3	1:E:195:ASP:HB2	1.74	0.69
1:A:214:ASN:HD22	1:A:214:ASN:N	1.88	0.69
1:B:121:VAL:CG1	1:C:123:GLN:HB3	2.23	0.69
1:D:300:GLY:H	1:D:323:SER:CB	2.01	0.68
1:D:292:GLU:HA	1:D:316:GLY:CA	2.20	0.68
1:A:292:GLU:HA	1:A:316:GLY:CA	2.21	0.68
1:F:292:GLU:HA	1:F:316:GLY:CA	2.20	0.68
1:F:398:ILE:HG12	1:F:426:ILE:CD1	2.24	0.68
1:A:391:GLU:OE2	1:A:420:LYS:HE3	1.93	0.68
1:B:295:LYS:HG2	1:B:318:ILE:HG21	1.74	0.68
1:E:358:LEU:HD11	1:E:366:TYR:HB3	1.74	0.68
1:C:292:GLU:HA	1:C:316:GLY:CA	2.23	0.68
1:A:246:LYS:HE3	1:B:214:ASN:ND2	2.09	0.67
1:D:390:ASN:HB2	1:D:393:ASP:OD1	1.94	0.67
1:B:123:GLN:HB3	1:C:121:VAL:CG1	2.25	0.67
1:A:128:TRP:HE1	1:A:138:ASN:HD22	1.42	0.67
1:B:295:LYS:HG2	1:B:318:ILE:CG2	2.24	0.67
1:B:128:TRP:HE1	1:B:138:ASN:HD22	1.42	0.67
1:F:329:ILE:CD1	1:F:357:TYR:HB3	2.24	0.67
1:D:121:VAL:HG13	1:F:123:GLN:HB3	1.77	0.67
1:A:300:GLY:N	1:A:323:SER:HB3	2.08	0.67
1:D:160:PRO:HG3	1:D:195:ASP:HB2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:GLY:N	1:B:323:SER:HB3	2.10	0.67
1:A:121:VAL:CG1	1:E:123:GLN:HB3	2.26	0.66
1:C:339:GLN:HB3	1:C:357:TYR:OH	1.95	0.66
1:E:214:ASN:ND2	1:F:246:LYS:HE3	2.10	0.66
1:D:214:ASN:HD22	1:D:214:ASN:N	1.92	0.66
1:D:128:TRP:HE1	1:D:138:ASN:HD22	1.43	0.66
1:B:390:ASN:ND2	1:B:391:GLU:H	1.94	0.66
1:A:123:GLN:HB3	1:E:121:VAL:CG1	2.25	0.65
1:E:128:TRP:HE1	1:E:138:ASN:HD22	1.42	0.65
1:E:329:ILE:HD13	1:E:357:TYR:HD2	1.62	0.65
1:B:105:ASP:OD1	1:B:107:VAL:HG23	1.97	0.65
1:F:430:PRO:CG	1:F:489:VAL:HA	2.25	0.65
1:D:346:ILE:HG23	1:D:352:LEU:HB2	1.79	0.65
1:A:121:VAL:HG13	1:E:123:GLN:HB3	1.78	0.65
1:B:259:ASN:ND2	1:B:260:ILE:H	1.94	0.65
1:F:384:ALA:HB3	1:F:388:GLU:CD	2.17	0.65
1:D:385:THR:HG22	1:D:386:GLN:N	2.13	0.64
1:C:346:ILE:CD1	1:C:357:TYR:HA	2.28	0.64
1:E:375:ILE:HG23	1:E:376:PRO:HD2	1.79	0.64
1:E:295:LYS:HD3	1:E:320:LEU:HD11	1.79	0.64
1:A:105:ASP:OD1	1:A:107:VAL:HG23	1.97	0.64
1:E:355:LYS:HE2	1:E:366:TYR:OH	1.98	0.64
1:A:123:GLN:HB3	1:E:121:VAL:HG13	1.78	0.64
1:C:128:TRP:HE1	1:C:138:ASN:HD22	1.43	0.64
1:E:259:ASN:ND2	1:E:260:ILE:H	1.94	0.64
1:E:300:GLY:N	1:E:323:SER:HB3	2.12	0.64
1:F:266:ASN:O	1:F:267:ILE:HB	1.98	0.64
1:B:117:GLU:HB3	1:C:125:ARG:HD3	1.79	0.64
1:F:55:LEU:HD23	1:F:55:LEU:O	1.97	0.63
1:F:105:ASP:OD1	1:F:107:VAL:HG23	1.98	0.63
1:D:259:ASN:ND2	1:D:260:ILE:H	1.95	0.63
1:A:329:ILE:HD11	1:A:354:LEU:O	1.98	0.63
1:F:398:ILE:HG12	1:F:426:ILE:HD12	1.81	0.63
1:E:387:ASN:OD1	1:E:414:HIS:HA	1.99	0.63
1:A:350:GLN:O	1:A:352:LEU:HG	1.99	0.63
1:D:159:HIS:HD2	1:D:161:ALA:HB3	1.63	0.63
1:F:400:ASN:O	1:F:401:LYS:HB2	1.97	0.63
1:F:128:TRP:HE1	1:F:138:ASN:HD22	1.45	0.63
1:E:390:ASN:HA	1:E:414:HIS:HB2	1.80	0.62
1:B:266:ASN:O	1:B:267:ILE:HB	1.99	0.62
1:E:266:ASN:O	1:E:267:ILE:HB	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:HIS:HD2	1:C:161:ALA:HB3	1.63	0.62
1:A:159:HIS:HD2	1:A:161:ALA:HB3	1.63	0.62
1:D:348:ASN:O	1:D:351:ARG:HD3	1.98	0.62
1:B:328:TYR:CD2	1:B:372:PRO:HB3	2.35	0.62
1:D:123:GLN:HB3	1:F:121:VAL:HG13	1.82	0.62
1:E:297:LEU:HD12	1:E:377:CYS:HB3	1.80	0.62
1:B:300:GLY:H	1:B:323:SER:HB3	1.62	0.62
1:C:259:ASN:ND2	1:C:260:ILE:H	1.97	0.62
1:E:159:HIS:HD2	1:E:161:ALA:HB3	1.65	0.62
1:C:284:LEU:HD11	1:C:379:ILE:HD11	1.81	0.62
1:F:390:ASN:HB2	1:F:393:ASP:OD2	1.99	0.62
1:F:159:HIS:HD2	1:F:161:ALA:HB3	1.63	0.62
1:D:266:ASN:O	1:D:267:ILE:HB	1.99	0.61
1:F:259:ASN:ND2	1:F:260:ILE:H	1.98	0.61
1:F:267:ILE:O	1:F:267:ILE:HG22	2.01	0.61
1:A:259:ASN:ND2	1:A:260:ILE:H	1.98	0.61
1:E:105:ASP:OD1	1:E:107:VAL:HG23	1.99	0.61
1:B:382:PRO:HB2	1:B:412:PRO:HB2	1.83	0.61
1:B:299:SER:HB3	1:B:382:PRO:HA	1.83	0.61
1:C:385:THR:HG22	1:C:386:GLN:H	1.66	0.61
1:A:65:SER:O	1:A:68:ASN:N	2.32	0.60
1:D:105:ASP:OD1	1:D:107:VAL:HG23	2.00	0.60
1:B:358:LEU:HD21	1:B:366:TYR:HB2	1.83	0.60
1:B:360:TYR:CD1	1:B:360:TYR:N	2.69	0.60
1:C:300:GLY:N	1:C:323:SER:HB3	2.06	0.60
1:A:266:ASN:O	1:A:267:ILE:HB	2.01	0.60
1:F:355:LYS:HG2	1:F:366:TYR:CZ	2.37	0.60
1:C:62:SER:OG	1:C:64:LYS:HG3	2.01	0.60
1:F:467:ILE:O	1:F:471:ILE:HG13	2.01	0.60
1:C:266:ASN:O	1:C:267:ILE:HB	2.01	0.60
1:A:306:GLN:OE1	1:A:344:MET:HG2	2.02	0.60
1:D:125:ARG:HD3	1:F:117:GLU:HB3	1.83	0.60
1:C:246:LYS:HE3	1:D:214:ASN:ND2	2.17	0.60
1:C:295:LYS:HA	1:C:318:ILE:HG22	1.84	0.60
1:C:306:GLN:OE1	1:C:344:MET:HG2	2.02	0.59
1:A:246:LYS:HE3	1:B:214:ASN:HD21	1.66	0.59
1:D:153:LYS:HE2	1:D:185:MET:HE2	1.83	0.59
1:D:385:THR:HG22	1:D:386:GLN:H	1.66	0.59
1:F:153:LYS:HE2	1:F:185:MET:HE2	1.85	0.59
1:D:339:GLN:NE2	1:D:357:TYR:OH	2.35	0.59
1:E:390:ASN:HA	1:E:414:HIS:CB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ILE:O	1:B:471:ILE:HG13	2.03	0.59
1:D:467:ILE:O	1:D:471:ILE:HG13	2.01	0.59
1:F:398:ILE:CG2	1:F:424:ASN:HB3	2.33	0.59
1:F:398:ILE:HD13	1:F:424:ASN:ND2	2.18	0.59
1:C:467:ILE:O	1:C:471:ILE:HG13	2.03	0.59
1:A:267:ILE:CG2	1:A:267:ILE:O	2.51	0.58
1:B:329:ILE:HD13	1:B:357:TYR:HD2	1.68	0.58
1:E:153:LYS:HE2	1:E:185:MET:HE2	1.86	0.58
1:A:178:ASN:O	1:A:181:THR:HB	2.03	0.58
1:A:212:MET:O	1:A:216:PHE:HB3	2.04	0.58
1:D:298:VAL:CG2	1:D:319:VAL:HG23	2.34	0.58
1:A:267:ILE:O	1:A:267:ILE:HG22	2.03	0.58
1:D:123:GLN:HB3	1:F:121:VAL:CG1	2.34	0.58
1:C:329:ILE:CD1	1:C:354:LEU:HG	2.33	0.58
1:C:105:ASP:OD1	1:C:107:VAL:HG23	2.04	0.58
1:B:159:HIS:HD2	1:B:161:ALA:HB3	1.66	0.58
1:A:64:LYS:HE2	1:A:72:GLU:OE1	2.02	0.58
1:E:277:VAL:CG2	1:E:308:LEU:HD12	2.31	0.58
1:F:267:ILE:HD11	1:F:461:ASP:HB2	1.86	0.58
1:D:306:GLN:OE1	1:D:344:MET:HG2	2.03	0.58
1:B:153:LYS:HG3	1:B:185:MET:CE	2.34	0.58
1:D:395:ASP:HA	1:D:398:ILE:HD12	1.86	0.58
1:D:394:ALA:O	1:D:398:ILE:HG13	2.03	0.58
1:E:214:ASN:HD21	1:F:246:LYS:HE3	1.69	0.57
1:B:318:ILE:HG22	1:B:318:ILE:O	2.04	0.57
1:A:467:ILE:O	1:A:471:ILE:HG13	2.04	0.57
1:C:355:LYS:C	1:C:357:TYR:H	2.08	0.57
1:B:159:HIS:HB3	1:B:162:VAL:HG23	1.86	0.57
1:A:153:LYS:HE2	1:A:185:MET:HE2	1.86	0.57
1:D:121:VAL:CG1	1:F:123:GLN:HB3	2.34	0.57
1:C:153:LYS:HE2	1:C:185:MET:HE2	1.86	0.57
1:B:258:LYS:NZ	1:B:449:ASN:HD21	2.03	0.57
1:F:178:ASN:O	1:F:181:THR:HB	2.03	0.57
1:C:178:ASN:O	1:C:181:THR:HB	2.04	0.57
1:D:280:ALA:HB2	1:D:406:VAL:HG21	1.87	0.57
1:E:280:ALA:HB2	1:E:406:VAL:HG21	1.86	0.57
1:E:60:TYR:N	1:E:60:TYR:CD1	2.73	0.57
1:F:306:GLN:OE1	1:F:344:MET:HG2	2.04	0.57
1:F:267:ILE:O	1:F:267:ILE:CG2	2.52	0.57
1:A:134:GLU:HG2	1:E:57:ASN:OD1	2.05	0.57
1:D:329:ILE:HD12	1:D:354:LEU:CG	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ASN:O	1:D:181:THR:HB	2.05	0.57
1:C:267:ILE:HG22	1:C:267:ILE:O	2.04	0.57
1:E:373:TRP:CE3	1:E:397:PHE:HZ	2.23	0.57
1:E:394:ALA:O	1:E:398:ILE:HG13	2.04	0.57
1:E:267:ILE:HD11	1:E:461:ASP:HB2	1.87	0.57
1:B:178:ASN:O	1:B:181:THR:HB	2.05	0.56
1:E:306:GLN:OE1	1:E:344:MET:HG2	2.05	0.56
1:E:318:ILE:HG22	1:E:318:ILE:O	2.06	0.56
1:C:159:HIS:HB3	1:C:162:VAL:HG23	1.87	0.56
1:A:65:SER:O	1:A:67:ASP:N	2.38	0.56
1:A:358:LEU:HD11	1:A:366:TYR:CB	2.35	0.56
1:D:63:THR:HG22	1:D:63:THR:O	2.05	0.56
1:B:328:TYR:CG	1:B:372:PRO:HB3	2.40	0.56
1:E:153:LYS:HG3	1:E:185:MET:CE	2.35	0.56
1:A:125:ARG:HD3	1:E:117:GLU:HB3	1.87	0.56
1:A:395:ASP:O	1:A:399:GLN:HB2	2.06	0.56
1:D:375:ILE:HD12	1:D:375:ILE:N	2.20	0.56
1:C:290:ASN:ND2	1:C:292:GLU:HB2	2.20	0.56
1:B:267:ILE:HG22	1:B:267:ILE:O	2.05	0.56
1:C:267:ILE:CG2	1:C:267:ILE:O	2.53	0.56
1:F:299:SER:O	1:F:383:CYS:HB2	2.06	0.56
1:E:159:HIS:HB3	1:E:162:VAL:HG23	1.86	0.56
1:F:159:HIS:HB3	1:F:162:VAL:HG23	1.87	0.56
1:D:267:ILE:CG2	1:D:267:ILE:O	2.54	0.56
1:D:318:ILE:HG22	1:D:318:ILE:O	2.06	0.56
1:B:205:LEU:O	1:B:209:GLN:HG3	2.05	0.56
1:F:121:VAL:HG23	1:F:143:VAL:HG22	1.88	0.56
1:D:267:ILE:O	1:D:267:ILE:HG22	2.05	0.56
1:F:181:THR:O	1:F:182:THR:CB	2.51	0.56
1:D:358:LEU:HD23	1:D:364:ALA:HB3	1.87	0.56
1:C:328:TYR:HD2	1:C:370:GLN:O	1.89	0.55
1:D:159:HIS:HB3	1:D:162:VAL:HG23	1.87	0.55
1:F:349:ASN:O	1:F:351:ARG:HG3	2.06	0.55
1:B:117:GLU:HG3	1:C:125:ARG:HB2	1.87	0.55
1:A:159:HIS:HB3	1:A:162:VAL:HG23	1.87	0.55
1:A:358:LEU:HD11	1:A:366:TYR:HB3	1.87	0.55
1:F:205:LEU:O	1:F:209:GLN:HG3	2.07	0.55
1:D:74:ARG:O	1:D:78:VAL:HG23	2.06	0.55
1:E:178:ASN:O	1:E:181:THR:HB	2.07	0.55
1:C:329:ILE:HD12	1:C:354:LEU:HG	1.88	0.55
1:A:332:PRO:O	1:A:333:ASN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:318:ILE:HG22	1:F:318:ILE:O	2.06	0.55
1:E:267:ILE:O	1:E:267:ILE:HG22	2.07	0.55
1:F:332:PRO:O	1:F:333:ASN:HB2	2.07	0.55
1:F:398:ILE:HG21	1:F:424:ASN:HB3	1.88	0.55
1:B:117:GLU:O	1:C:125:ARG:NH1	2.39	0.55
1:B:60:TYR:O	1:B:61:THR:HG23	2.06	0.55
1:C:267:ILE:HD11	1:C:461:ASP:HB2	1.89	0.55
1:D:290:ASN:ND2	1:D:292:GLU:HB2	2.20	0.55
1:D:134:GLU:HG2	1:F:57:ASN:ND2	2.22	0.55
1:F:153:LYS:HG3	1:F:185:MET:CE	2.37	0.55
1:D:212:MET:O	1:D:216:PHE:HB3	2.07	0.55
1:D:181:THR:O	1:D:182:THR:CB	2.54	0.54
1:C:318:ILE:O	1:C:318:ILE:HG22	2.06	0.54
1:C:332:PRO:O	1:C:333:ASN:HB2	2.08	0.54
1:E:457:HIS:HB2	2:E:534:HOH:O	2.06	0.54
1:A:329:ILE:CD1	1:A:354:LEU:HG	2.36	0.54
1:B:74:ARG:O	1:B:78:VAL:HG23	2.07	0.54
1:F:280:ALA:HB2	1:F:406:VAL:HG21	1.89	0.54
1:C:205:LEU:O	1:C:209:GLN:HG3	2.06	0.54
1:B:280:ALA:HB2	1:B:406:VAL:HG21	1.88	0.54
1:C:369:ASN:O	1:C:370:GLN:HG3	2.07	0.54
1:F:352:LEU:HD13	1:F:356:GLU:HG3	1.89	0.54
1:F:351:ARG:CB	1:F:351:ARG:HH11	2.19	0.54
1:D:385:THR:HG23	1:D:386:GLN:HE21	1.72	0.54
1:E:329:ILE:HD13	1:E:357:TYR:CD2	2.40	0.54
1:D:125:ARG:NH1	1:F:117:GLU:O	2.40	0.54
1:F:277:VAL:CG2	1:F:308:LEU:HD12	2.37	0.54
1:A:300:GLY:H	1:A:323:SER:CB	2.19	0.54
1:C:328:TYR:CE1	1:C:372:PRO:HB3	2.42	0.54
1:A:121:VAL:HG23	1:A:143:VAL:HG22	1.88	0.54
1:E:121:VAL:HG23	1:E:143:VAL:HG22	1.90	0.54
1:D:352:LEU:HB3	1:D:356:GLU:HG3	1.89	0.54
1:D:332:PRO:O	1:D:333:ASN:HB2	2.08	0.54
1:E:60:TYR:HB3	1:E:69:GLN:NE2	2.23	0.54
1:F:74:ARG:O	1:F:78:VAL:HG23	2.07	0.54
1:D:385:THR:HG22	1:D:386:GLN:HG2	1.88	0.54
1:A:318:ILE:HG22	1:A:318:ILE:O	2.07	0.54
1:B:306:GLN:OE1	1:B:344:MET:HG2	2.08	0.54
1:B:267:ILE:CG2	1:B:267:ILE:O	2.56	0.54
1:C:346:ILE:HD11	1:C:357:TYR:HA	1.90	0.53
1:E:375:ILE:CG2	1:E:376:PRO:HD2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ALA:HB2	1:A:406:VAL:HG21	1.90	0.53
1:A:258:LYS:NZ	1:A:449:ASN:HD21	2.06	0.53
1:C:394:ALA:HB1	1:C:421:LEU:HG	1.90	0.53
1:E:295:LYS:CD	1:E:320:LEU:HD11	2.38	0.53
1:B:153:LYS:HE2	1:B:185:MET:HE2	1.90	0.53
1:C:74:ARG:O	1:C:78:VAL:HG23	2.08	0.53
1:B:332:PRO:O	1:B:333:ASN:HB2	2.07	0.53
1:E:396:LEU:O	1:E:400:ASN:ND2	2.41	0.53
1:C:258:LYS:NZ	1:C:449:ASN:HD21	2.06	0.53
1:E:205:LEU:O	1:E:209:GLN:HG3	2.09	0.53
1:F:212:MET:O	1:F:216:PHE:HB3	2.08	0.53
1:A:74:ARG:O	1:A:78:VAL:HG23	2.07	0.53
1:B:351:ARG:HB3	1:B:351:ARG:CZ	2.39	0.53
1:A:181:THR:O	1:A:182:THR:CB	2.55	0.53
1:F:258:LYS:NZ	1:F:449:ASN:HD21	2.07	0.53
1:C:280:ALA:HB2	1:C:406:VAL:HG21	1.91	0.53
1:E:267:ILE:O	1:E:267:ILE:CG2	2.55	0.53
1:C:302:GLY:O	1:C:306:GLN:HG3	2.08	0.53
1:C:258:LYS:HZ1	1:C:449:ASN:HD21	1.56	0.53
1:A:153:LYS:HG3	1:A:185:MET:CE	2.39	0.53
1:A:267:ILE:HD11	1:A:461:ASP:HB2	1.91	0.52
1:E:170:LEU:HB3	1:E:189:LYS:HE2	1.91	0.52
1:C:401:LYS:HZ3	1:C:401:LYS:HA	1.70	0.52
1:A:205:LEU:O	1:A:209:GLN:HG3	2.08	0.52
1:B:384:ALA:N	1:B:388:GLU:OE2	2.42	0.52
1:B:290:ASN:ND2	1:B:292:GLU:HB2	2.20	0.52
1:C:121:VAL:HG23	1:C:143:VAL:HG22	1.92	0.52
1:E:355:LYS:HG2	1:E:366:TYR:CE2	2.43	0.52
1:D:121:VAL:HG23	1:D:143:VAL:HG22	1.91	0.52
1:D:205:LEU:O	1:D:209:GLN:HG3	2.09	0.52
1:E:299:SER:HB3	1:E:382:PRO:HA	1.91	0.52
1:B:421:LEU:HD23	1:B:426:ILE:HD12	1.91	0.52
1:E:290:ASN:ND2	1:E:292:GLU:HB2	2.20	0.52
1:B:358:LEU:HD21	1:B:366:TYR:CB	2.40	0.52
1:B:382:PRO:HB2	1:B:412:PRO:CB	2.39	0.52
1:D:298:VAL:CG1	1:D:308:LEU:HD23	2.39	0.52
1:B:351:ARG:NH1	1:B:351:ARG:HB3	2.24	0.52
1:E:370:GLN:HE21	1:E:374:ASN:HD21	1.58	0.52
1:D:328:TYR:HD2	1:D:370:GLN:O	1.93	0.52
1:D:421:LEU:HD23	1:D:426:ILE:HD12	1.92	0.52
1:B:181:THR:O	1:B:182:THR:CB	2.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:LYS:HG2	1:E:366:TYR:CZ	2.44	0.52
1:E:212:MET:O	1:E:216:PHE:HB3	2.09	0.52
1:A:290:ASN:ND2	1:A:292:GLU:HB2	2.20	0.51
1:C:277:VAL:CG2	1:C:308:LEU:HD12	2.39	0.51
1:F:398:ILE:HA	1:F:426:ILE:HD11	1.91	0.51
1:E:397:PHE:HD2	1:E:402:CYS:HG	1.54	0.51
1:E:58:TYR:OH	1:E:509:GLY:HA3	2.10	0.51
1:C:346:ILE:HG23	1:C:352:LEU:HB2	1.91	0.51
1:C:385:THR:HG22	1:C:386:GLN:N	2.24	0.51
1:B:406:VAL:HA	1:B:429:CYS:HB2	1.92	0.51
1:C:153:LYS:HG3	1:C:185:MET:CE	2.40	0.51
1:F:406:VAL:HA	1:F:429:CYS:HB2	1.91	0.51
1:B:342:TYR:O	1:B:346:ILE:HG13	2.11	0.51
1:D:258:LYS:NZ	1:D:449:ASN:HD21	2.09	0.51
1:F:350:GLN:CB	1:F:352:LEU:HD11	2.37	0.51
1:C:214:ASN:ND2	1:D:246:LYS:HE3	2.25	0.51
1:F:421:LEU:HD23	1:F:426:ILE:HD12	1.92	0.51
1:B:267:ILE:HD11	1:B:461:ASP:HB2	1.91	0.51
1:C:66:VAL:O	1:C:70:ILE:HG13	2.11	0.51
1:A:398:ILE:HD13	1:A:424:ASN:ND2	2.25	0.51
1:A:346:ILE:HA	1:A:350:GLN:HB2	1.91	0.51
1:B:391:GLU:O	1:B:394:ALA:HB3	2.10	0.51
1:E:74:ARG:O	1:E:78:VAL:HG23	2.10	0.51
1:E:294:LYS:O	1:E:318:ILE:HB	2.10	0.51
1:D:298:VAL:HG23	1:D:319:VAL:HG23	1.92	0.51
1:A:214:ASN:ND2	1:A:214:ASN:N	2.59	0.51
1:D:267:ILE:HD11	1:D:461:ASP:HB2	1.92	0.51
1:F:418:LEU:HD23	1:F:418:LEU:O	2.11	0.51
1:E:297:LEU:HG	1:E:377:CYS:CB	2.39	0.51
1:E:259:ASN:ND2	1:E:260:ILE:N	2.59	0.51
1:E:406:VAL:HA	1:E:429:CYS:HB2	1.92	0.51
1:C:214:ASN:N	1:C:214:ASN:ND2	2.59	0.50
1:E:467:ILE:O	1:E:471:ILE:HG13	2.11	0.50
1:A:374:ASN:HA	1:A:396:LEU:HD22	1.93	0.50
1:E:258:LYS:NZ	1:E:449:ASN:HD21	2.08	0.50
1:B:259:ASN:ND2	1:B:260:ILE:N	2.59	0.50
1:D:60:TYR:HE2	1:D:109:ILE:HG22	1.75	0.50
1:D:61:THR:HG22	1:D:61:THR:O	2.11	0.50
1:C:181:THR:O	1:C:182:THR:CB	2.55	0.50
1:D:277:VAL:CG2	1:D:308:LEU:HD12	2.38	0.50
1:F:375:ILE:N	1:F:375:ILE:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PRO:HG3	1:A:195:ASP:CB	2.40	0.50
1:F:398:ILE:HG12	1:F:426:ILE:HD11	1.93	0.50
1:E:397:PHE:HD2	1:E:402:CYS:SG	2.35	0.50
1:B:384:ALA:HB3	1:B:388:GLU:OE2	2.12	0.50
1:B:130:ASN:ND2	1:B:134:GLU:HB2	2.26	0.50
1:C:298:VAL:O	1:C:322:MET:HA	2.12	0.50
1:F:329:ILE:HG21	1:F:357:TYR:CD2	2.47	0.50
1:C:330:LEU:HG	1:C:332:PRO:HD3	1.94	0.50
1:A:406:VAL:HA	1:A:429:CYS:HB2	1.93	0.50
1:C:406:VAL:HA	1:C:429:CYS:HB2	1.93	0.50
1:D:66:VAL:O	1:D:70:ILE:HG13	2.12	0.50
1:E:301:SER:OG	1:E:347:LYS:HE2	2.12	0.50
1:F:66:VAL:O	1:F:70:ILE:HG13	2.11	0.50
1:E:302:GLY:O	1:E:306:GLN:HG3	2.12	0.50
1:F:130:ASN:ND2	1:F:134:GLU:HB2	2.27	0.50
1:B:302:GLY:O	1:B:306:GLN:HG3	2.12	0.49
1:E:378:ASP:N	1:E:378:ASP:OD1	2.44	0.49
1:D:259:ASN:ND2	1:D:260:ILE:N	2.60	0.49
1:B:360:TYR:N	1:B:360:TYR:HD1	2.10	0.49
1:D:339:GLN:CD	1:D:357:TYR:OH	2.51	0.49
1:C:373:TRP:HA	1:C:373:TRP:CE3	2.47	0.49
1:C:430:PRO:HG3	1:C:489:VAL:CA	2.39	0.49
1:B:358:LEU:HD11	1:B:366:TYR:CB	2.42	0.49
1:E:342:TYR:O	1:E:346:ILE:HG13	2.12	0.49
1:B:384:ALA:HB3	1:B:388:GLU:CD	2.32	0.49
1:D:342:TYR:O	1:D:346:ILE:HG13	2.13	0.49
1:F:358:LEU:HD11	1:F:366:TYR:HB3	1.94	0.49
1:F:153:LYS:HE2	1:F:185:MET:CE	2.42	0.49
1:B:212:MET:O	1:B:216:PHE:HB3	2.13	0.49
1:D:298:VAL:HG11	1:D:308:LEU:HD23	1.94	0.49
1:C:355:LYS:HE3	1:C:366:TYR:CD2	2.48	0.49
1:B:295:LYS:HA	1:B:318:ILE:HG22	1.93	0.49
1:E:291:LEU:O	1:E:294:LYS:HG2	2.12	0.49
1:A:66:VAL:O	1:A:70:ILE:HG13	2.12	0.49
1:A:63:THR:O	1:A:64:LYS:O	2.29	0.49
1:C:373:TRP:HA	1:C:373:TRP:HE3	1.78	0.49
1:E:246:LYS:HE3	1:F:214:ASN:ND2	2.27	0.49
1:D:153:LYS:HG3	1:D:185:MET:CE	2.42	0.49
1:A:339:GLN:NE2	1:A:357:TYR:OH	2.46	0.49
1:C:160:PRO:HG3	1:C:195:ASP:CB	2.41	0.49
1:C:258:LYS:HZ1	1:C:449:ASN:ND2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:GLN:C	1:B:351:ARG:HG2	2.33	0.49
1:A:421:LEU:HD23	1:A:426:ILE:HD12	1.94	0.49
1:B:324:ASP:HB2	1:B:354:LEU:HD22	1.95	0.49
1:E:330:LEU:HG	1:E:332:PRO:HD3	1.94	0.48
1:A:214:ASN:ND2	1:B:246:LYS:HE3	2.27	0.48
1:F:291:LEU:O	1:F:294:LYS:HG2	2.13	0.48
1:A:258:LYS:HZ1	1:A:449:ASN:HD21	1.58	0.48
1:F:502:ASP:O	1:F:506:GLU:HG3	2.13	0.48
1:E:66:VAL:O	1:E:70:ILE:HG13	2.13	0.48
1:E:214:ASN:N	1:E:214:ASN:ND2	2.60	0.48
1:E:332:PRO:O	1:E:333:ASN:HB2	2.12	0.48
1:A:391:GLU:O	1:A:394:ALA:N	2.44	0.48
1:B:153:LYS:HG3	1:B:185:MET:HE3	1.95	0.48
1:F:302:GLY:O	1:F:306:GLN:HG3	2.14	0.48
1:B:385:THR:O	1:B:388:GLU:HG3	2.12	0.48
1:E:421:LEU:HD23	1:E:426:ILE:HD12	1.95	0.48
1:C:421:LEU:HD23	1:C:426:ILE:HD12	1.95	0.48
1:F:214:ASN:N	1:F:214:ASN:ND2	2.60	0.48
1:E:153:LYS:HE2	1:E:185:MET:CE	2.43	0.48
1:B:375:ILE:HG23	1:B:376:PRO:HD2	1.94	0.48
1:E:159:HIS:O	1:E:193:ASP:HA	2.13	0.48
1:D:125:ARG:HB2	1:F:117:GLU:HG3	1.94	0.48
1:D:65:SER:OG	1:D:68:ASN:ND2	2.47	0.48
1:B:270:GLU:HB3	1:B:307:TYR:CD2	2.48	0.48
1:B:430:PRO:HG3	1:B:489:VAL:CA	2.39	0.48
1:A:368:GLU:HG2	1:A:369:ASN:N	2.29	0.48
1:C:212:MET:O	1:C:216:PHE:HB3	2.13	0.48
1:B:293:ASN:C	1:B:318:ILE:HD12	2.34	0.48
1:A:125:ARG:HB2	1:E:117:GLU:HG3	1.96	0.48
1:D:73:LEU:CD1	1:D:113:GLU:HG3	2.44	0.48
1:F:259:ASN:ND2	1:F:260:ILE:N	2.62	0.48
1:B:349:ASN:O	1:B:351:ARG:HG2	2.13	0.48
1:E:258:LYS:HZ1	1:E:449:ASN:HD21	1.61	0.48
1:E:326:ASN:HD21	1:E:355:LYS:HE3	1.78	0.47
1:E:397:PHE:CD2	1:E:402:CYS:SG	3.07	0.47
1:B:83:ASN:C	1:B:85:PRO:HD3	2.35	0.47
1:F:290:ASN:ND2	1:F:292:GLU:HB2	2.22	0.47
1:E:181:THR:O	1:E:182:THR:CB	2.55	0.47
1:E:373:TRP:HA	1:E:373:TRP:CE3	2.49	0.47
1:D:294:LYS:O	1:D:318:ILE:HB	2.14	0.47
1:D:295:LYS:HA	1:D:318:ILE:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:LEU:HG	1:D:332:PRO:HD3	1.95	0.47
1:B:258:LYS:HZ1	1:B:449:ASN:HD21	1.61	0.47
1:A:330:LEU:HG	1:A:332:PRO:HD3	1.95	0.47
1:F:330:LEU:HG	1:F:332:PRO:HD3	1.96	0.47
1:A:376:PRO:CA	1:A:400:ASN:HD22	2.27	0.47
1:C:418:LEU:O	1:C:418:LEU:HD23	2.14	0.47
1:D:406:VAL:HA	1:D:429:CYS:HB2	1.95	0.47
1:C:367:PHE:O	1:C:368:GLU:C	2.52	0.47
1:A:153:LYS:HE2	1:A:185:MET:CE	2.44	0.47
1:E:83:ASN:C	1:E:85:PRO:HD3	2.34	0.47
1:C:355:LYS:HG3	1:C:366:TYR:CD2	2.49	0.47
1:D:342:TYR:CD1	1:D:360:TYR:HB3	2.50	0.47
1:C:259:ASN:ND2	1:C:260:ILE:N	2.62	0.47
1:E:373:TRP:CE3	1:E:397:PHE:CZ	3.03	0.47
1:B:121:VAL:HG23	1:B:143:VAL:HG22	1.95	0.47
1:E:502:ASP:O	1:E:506:GLU:HG3	2.14	0.47
1:E:380:ALA:HB3	1:E:405:ILE:HG12	1.96	0.47
1:B:58:TYR:HB3	1:B:59:GLY:H	1.52	0.47
1:F:300:GLY:H	1:F:323:SER:CB	2.21	0.47
1:B:159:HIS:O	1:B:193:ASP:HA	2.15	0.47
1:A:130:ASN:ND2	1:A:134:GLU:HB2	2.30	0.47
1:E:383:CYS:HA	1:E:409:ALA:HB2	1.96	0.47
1:D:258:LYS:HZ1	1:D:449:ASN:HD21	1.63	0.47
1:B:66:VAL:O	1:B:70:ILE:HG13	2.15	0.47
1:E:300:GLY:H	1:E:323:SER:CB	2.15	0.47
1:D:430:PRO:HG3	1:D:489:VAL:CA	2.40	0.47
1:C:343:ILE:HG23	1:C:354:LEU:CD1	2.45	0.47
1:A:83:ASN:C	1:A:85:PRO:HD3	2.35	0.47
1:E:386:GLN:O	1:E:387:ASN:C	2.52	0.47
1:A:259:ASN:ND2	1:A:260:ILE:N	2.62	0.47
1:C:452:ARG:NH2	1:F:221:PRO:O	2.48	0.47
1:D:170:LEU:HB3	1:D:189:LYS:HE2	1.97	0.47
1:A:277:VAL:CG2	1:A:308:LEU:HD12	2.39	0.47
1:C:328:TYR:CD2	1:C:372:PRO:HD3	2.49	0.47
1:E:352:LEU:O	1:E:353:ARG:C	2.53	0.47
1:B:73:LEU:CD1	1:B:113:GLU:HG3	2.45	0.47
1:E:293:ASN:C	1:E:318:ILE:HD12	2.36	0.46
1:B:330:LEU:HG	1:B:332:PRO:HD3	1.97	0.46
1:E:328:TYR:OH	1:E:375:ILE:HD11	2.14	0.46
1:A:159:HIS:O	1:A:193:ASP:HA	2.15	0.46
1:F:73:LEU:CD1	1:F:113:GLU:HG3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLY:O	1:A:306:GLN:HG3	2.15	0.46
1:C:295:LYS:HA	1:C:318:ILE:CG2	2.45	0.46
1:B:386:GLN:NE2	1:B:410:ASN:O	2.48	0.46
1:A:430:PRO:HG3	1:A:489:VAL:CA	2.39	0.46
1:D:298:VAL:HG13	1:D:381:PHE:HB2	1.98	0.46
1:B:294:LYS:O	1:B:318:ILE:HB	2.16	0.46
1:D:291:LEU:O	1:D:294:LYS:HG2	2.15	0.46
1:A:294:LYS:O	1:A:318:ILE:HB	2.14	0.46
1:C:147:SER:HB3	1:C:152:TYR:CE1	2.50	0.46
1:D:329:ILE:HD11	1:D:354:LEU:HG	1.89	0.46
1:E:328:TYR:O	1:E:366:TYR:HA	2.14	0.46
1:C:386:GLN:O	1:C:387:ASN:HB2	2.16	0.46
1:E:373:TRP:HA	1:E:373:TRP:HE3	1.79	0.46
1:F:301:SER:OG	1:F:347:LYS:HE2	2.15	0.46
1:B:395:ASP:O	1:B:398:ILE:HG12	2.16	0.46
1:A:65:SER:C	1:A:67:ASP:N	2.69	0.46
1:E:382:PRO:HB2	1:E:412:PRO:HB2	1.98	0.46
1:C:58:TYR:OH	1:C:509:GLY:HA3	2.15	0.46
1:E:130:ASN:ND2	1:E:134:GLU:HB2	2.31	0.46
1:E:430:PRO:HG3	1:E:489:VAL:CA	2.37	0.46
1:C:258:LYS:HB3	1:C:262:TRP:CZ3	2.51	0.46
1:F:342:TYR:O	1:F:346:ILE:HG13	2.14	0.46
1:D:160:PRO:HG3	1:D:195:ASP:CB	2.45	0.46
1:E:389:ILE:HG23	1:E:393:ASP:HB2	1.97	0.46
1:A:342:TYR:O	1:A:346:ILE:HG13	2.16	0.46
1:D:153:LYS:HE2	1:D:185:MET:CE	2.44	0.46
1:A:258:LYS:HZ1	1:A:449:ASN:ND2	2.14	0.46
1:E:145:TYR:CD2	1:E:175:ILE:HD11	2.51	0.46
1:F:329:ILE:HD13	1:F:357:TYR:CD2	2.51	0.46
1:C:159:HIS:O	1:C:193:ASP:HA	2.16	0.46
1:B:160:PRO:HG3	1:B:195:ASP:CB	2.44	0.46
1:F:159:HIS:O	1:F:193:ASP:HA	2.16	0.46
1:C:294:LYS:O	1:C:318:ILE:HB	2.16	0.46
1:F:372:PRO:O	1:F:375:ILE:HD13	2.16	0.46
1:C:73:LEU:CD1	1:C:113:GLU:HG3	2.46	0.46
1:D:117:GLU:O	1:F:125:ARG:NH1	2.49	0.46
1:A:418:LEU:O	1:A:418:LEU:HD23	2.16	0.46
1:B:401:LYS:HD2	1:B:401:LYS:N	2.31	0.46
1:F:398:ILE:HD13	1:F:424:ASN:CG	2.36	0.45
1:A:285:LYS:O	1:A:285:LYS:HG2	2.16	0.45
1:B:214:ASN:N	1:B:214:ASN:ND2	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:ASN:C	1:F:85:PRO:HD3	2.37	0.45
1:A:361:SER:CB	1:A:364:ALA:HB2	2.41	0.45
1:A:65:SER:O	1:A:66:VAL:C	2.54	0.45
1:F:358:LEU:HD11	1:F:366:TYR:CB	2.47	0.45
1:C:130:ASN:ND2	1:C:134:GLU:HB2	2.31	0.45
1:D:159:HIS:O	1:D:193:ASP:HA	2.16	0.45
1:E:73:LEU:CD1	1:E:113:GLU:HG3	2.47	0.45
1:F:99:LYS:HE2	1:F:103:LYS:HE3	1.98	0.45
1:F:63:THR:O	1:F:63:THR:HG22	2.16	0.45
1:B:60:TYR:CE1	1:B:109:ILE:HG22	2.52	0.45
1:F:170:LEU:HB3	1:F:189:LYS:HE2	1.98	0.45
1:C:502:ASP:O	1:C:506:GLU:HG3	2.16	0.45
1:D:502:ASP:O	1:D:506:GLU:HG3	2.16	0.45
1:B:62:SER:O	1:B:63:THR:HB	2.17	0.45
1:A:301:SER:OG	1:A:347:LYS:HE2	2.17	0.45
1:B:418:LEU:O	1:B:418:LEU:HD23	2.16	0.45
1:F:285:LYS:HG2	1:F:285:LYS:O	2.17	0.45
1:A:145:TYR:CD2	1:A:175:ILE:HD11	2.52	0.45
1:C:328:TYR:O	1:C:366:TYR:CD1	2.70	0.45
1:A:346:ILE:HG21	1:A:356:GLU:HB3	1.99	0.45
1:D:409:ALA:O	1:D:412:PRO:HD3	2.17	0.45
1:A:73:LEU:CD1	1:A:113:GLU:HG3	2.46	0.45
1:D:296:CYS:HA	1:D:379:ILE:O	2.17	0.45
1:C:297:LEU:HD23	1:C:320:LEU:HB2	1.99	0.45
1:F:401:LYS:O	1:F:402:CYS:C	2.55	0.45
1:F:397:PHE:O	1:F:402:CYS:HB3	2.16	0.45
1:E:153:LYS:HG3	1:E:185:MET:HE3	1.99	0.45
1:D:60:TYR:CE2	1:D:109:ILE:HG22	2.51	0.45
1:F:329:ILE:CD1	1:F:354:LEU:HG	2.47	0.44
1:F:160:PRO:HG3	1:F:195:ASP:CB	2.40	0.44
1:B:355:LYS:O	1:B:358:LEU:HD12	2.17	0.44
1:D:418:LEU:HD23	1:D:418:LEU:O	2.16	0.44
1:E:350:GLN:O	1:E:352:LEU:HG	2.17	0.44
1:D:429:CYS:HA	1:D:430:PRO:HD3	1.86	0.44
1:F:294:LYS:O	1:F:318:ILE:HB	2.17	0.44
1:F:397:PHE:CD1	1:F:405:ILE:HD11	2.52	0.44
1:E:400:ASN:O	1:E:401:LYS:HB3	2.18	0.44
1:C:270:GLU:HB3	1:C:307:TYR:CD2	2.52	0.44
1:C:83:ASN:C	1:C:85:PRO:HD3	2.37	0.44
1:B:285:LYS:HG2	1:B:285:LYS:O	2.18	0.44
1:D:343:ILE:HG23	1:D:354:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:TYR:O	1:C:346:ILE:HG13	2.17	0.44
1:D:130:ASN:ND2	1:D:134:GLU:HB2	2.33	0.44
1:A:246:LYS:CE	1:B:214:ASN:HD21	2.28	0.44
1:B:78:VAL:HA	1:B:88:LEU:HD21	1.99	0.44
1:D:385:THR:CG2	1:D:386:GLN:N	2.80	0.44
1:D:153:LYS:HD2	1:D:225:VAL:O	2.17	0.44
1:A:153:LYS:HD2	1:A:225:VAL:O	2.17	0.44
1:F:293:ASN:C	1:F:318:ILE:HD12	2.38	0.44
1:C:301:SER:OG	1:C:347:LYS:HE2	2.18	0.44
1:B:327:GLY:HA3	1:B:367:PHE:O	2.17	0.44
1:E:379:ILE:HA	1:E:404:MET:O	2.18	0.44
1:D:154:GLY:HA3	1:D:188:GLY:O	2.17	0.44
1:C:170:LEU:HB3	1:C:189:LYS:HE2	1.98	0.44
1:B:394:ALA:HA	1:B:397:PHE:HD1	1.82	0.44
1:A:291:LEU:O	1:A:294:LYS:HG2	2.18	0.44
1:B:502:ASP:O	1:B:506:GLU:HG3	2.17	0.44
1:D:270:GLU:HB3	1:D:307:TYR:CD2	2.53	0.44
1:A:380:ALA:O	1:A:382:PRO:HD3	2.18	0.44
1:B:99:LYS:N	1:B:100:PRO:CD	2.81	0.44
1:B:295:LYS:CG	1:B:318:ILE:HG21	2.46	0.44
1:E:295:LYS:HA	1:E:318:ILE:HG22	1.99	0.44
1:A:468:MET:CE	1:A:471:ILE:HD12	2.48	0.44
1:C:153:LYS:HD2	1:C:225:VAL:O	2.17	0.44
1:A:376:PRO:HG3	1:A:400:ASN:ND2	2.33	0.44
1:F:398:ILE:HG21	1:F:424:ASN:CB	2.48	0.44
1:D:371:LYS:NZ	1:D:390:ASN:ND2	2.66	0.44
1:A:63:THR:O	1:A:64:LYS:C	2.55	0.44
1:D:375:ILE:H	1:D:375:ILE:HD12	1.82	0.44
1:D:301:SER:OG	1:D:347:LYS:HE2	2.18	0.44
1:F:498:LEU:HD23	1:F:498:LEU:HA	1.87	0.44
1:B:277:VAL:CG2	1:B:308:LEU:HD12	2.41	0.43
1:A:352:LEU:HD13	1:A:356:GLU:OE1	2.18	0.43
1:F:258:LYS:HZ1	1:F:449:ASN:HD21	1.63	0.43
1:D:83:ASN:C	1:D:85:PRO:HD3	2.38	0.43
1:C:296:CYS:HA	1:C:379:ILE:O	2.17	0.43
1:B:356:GLU:O	1:B:360:TYR:CE1	2.71	0.43
1:C:153:LYS:HE2	1:C:185:MET:CE	2.47	0.43
1:F:418:LEU:HD23	1:F:418:LEU:C	2.37	0.43
1:F:58:TYR:OH	1:F:509:GLY:HA3	2.19	0.43
1:D:90:ALA:HB2	1:D:169:PHE:HD1	1.83	0.43
1:D:99:LYS:N	1:D:100:PRO:CD	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:LYS:HG2	1:E:285:LYS:O	2.17	0.43
1:C:217:ARG:HB2	1:C:217:ARG:CZ	2.49	0.43
1:C:366:TYR:C	1:C:367:PHE:HD1	2.22	0.43
1:D:302:GLY:O	1:D:306:GLN:HG3	2.17	0.43
1:C:291:LEU:O	1:C:294:LYS:HG2	2.17	0.43
1:A:295:LYS:HA	1:A:318:ILE:HG22	2.00	0.43
1:B:99:LYS:HE2	1:B:103:LYS:HE3	2.00	0.43
1:A:217:ARG:HB2	1:A:217:ARG:CZ	2.48	0.43
1:A:389:ILE:HG22	1:A:389:ILE:O	2.18	0.43
1:C:352:LEU:HB3	1:C:356:GLU:HG3	2.01	0.43
1:C:468:MET:CE	1:C:471:ILE:HD12	2.48	0.43
1:E:99:LYS:N	1:E:100:PRO:CD	2.81	0.43
1:B:293:ASN:HA	1:B:318:ILE:CD1	2.49	0.43
1:B:153:LYS:HE2	1:B:185:MET:CE	2.48	0.43
1:C:63:THR:HG22	1:C:63:THR:O	2.17	0.43
1:D:403:LYS:HB3	1:D:403:LYS:HE2	1.89	0.43
1:E:418:LEU:HD23	1:E:418:LEU:O	2.19	0.43
1:A:146:ASN:HD21	1:A:148:VAL:HB	1.84	0.43
1:F:145:TYR:CD2	1:F:175:ILE:HD11	2.54	0.43
1:A:224:ASP:O	1:A:226:PRO:HD3	2.19	0.43
1:E:153:LYS:HD2	1:E:225:VAL:O	2.19	0.43
1:D:365:LYS:HG2	1:D:367:PHE:CE1	2.54	0.43
1:F:336:THR:O	1:F:337:LYS:C	2.56	0.43
1:E:389:ILE:O	1:E:414:HIS:HB2	2.19	0.43
1:B:360:TYR:H	1:B:360:TYR:HD1	1.66	0.43
1:F:78:VAL:HA	1:F:88:LEU:HD21	2.00	0.43
1:C:99:LYS:HE2	1:C:103:LYS:HE3	2.00	0.43
1:B:145:TYR:CD2	1:B:175:ILE:HD11	2.54	0.43
1:D:285:LYS:HG2	1:D:285:LYS:O	2.19	0.43
1:C:392:ASN:N	1:C:392:ASN:HD22	2.16	0.43
1:A:99:LYS:HE2	1:A:103:LYS:HE3	2.01	0.43
1:A:366:TYR:HE2	1:A:368:GLU:HB2	1.84	0.43
1:C:216:PHE:CD2	1:C:247:LEU:HD13	2.54	0.43
1:F:451:MET:HE1	1:F:455:TRP:HE1	1.84	0.43
1:C:355:LYS:HE3	1:C:366:TYR:CE2	2.53	0.42
1:C:321:THR:HG21	1:C:372:PRO:HB2	2.01	0.42
1:A:394:ALA:O	1:A:398:ILE:HG13	2.17	0.42
1:B:367:PHE:CD1	1:B:367:PHE:N	2.87	0.42
1:D:90:ALA:HB2	1:D:169:PHE:CD1	2.54	0.42
1:C:217:ARG:NH1	1:C:217:ARG:HB2	2.34	0.42
1:C:99:LYS:N	1:C:100:PRO:CD	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ASP:O	1:B:226:PRO:HD3	2.19	0.42
1:D:339:GLN:HE21	1:D:361:SER:HB2	1.83	0.42
1:D:468:MET:CE	1:D:471:ILE:HD12	2.49	0.42
1:A:418:LEU:C	1:A:418:LEU:HD23	2.40	0.42
1:F:270:GLU:HB3	1:F:307:TYR:CD2	2.54	0.42
1:C:409:ALA:O	1:C:412:PRO:HD3	2.19	0.42
1:B:498:LEU:HD23	1:B:498:LEU:HA	1.89	0.42
1:A:502:ASP:O	1:A:506:GLU:HG3	2.20	0.42
1:E:160:PRO:HG3	1:E:195:ASP:CB	2.45	0.42
1:A:217:ARG:NH1	1:A:217:ARG:CB	2.82	0.42
1:A:217:ARG:NH1	1:A:217:ARG:HB2	2.35	0.42
1:B:217:ARG:NH1	1:B:217:ARG:HB2	2.34	0.42
1:A:409:ALA:O	1:A:412:PRO:HD3	2.18	0.42
1:D:306:GLN:HE22	1:D:348:ASN:HD21	1.65	0.42
1:B:261:LYS:HD2	1:E:506:GLU:OE1	2.20	0.42
1:F:469:LYS:O	1:F:473:GLU:HG3	2.19	0.42
1:B:170:LEU:HB3	1:B:189:LYS:HE2	2.00	0.42
1:F:382:PRO:HG2	1:F:407:GLU:HA	2.02	0.42
1:C:350:GLN:O	1:C:352:LEU:N	2.52	0.42
1:E:153:LYS:HG3	1:E:185:MET:HE2	2.00	0.42
1:A:170:LEU:HB3	1:A:189:LYS:HE2	2.01	0.42
1:D:146:ASN:HD21	1:D:148:VAL:HB	1.84	0.42
1:C:418:LEU:C	1:C:418:LEU:HD23	2.40	0.42
1:D:99:LYS:HE2	1:D:103:LYS:HE3	2.00	0.42
1:A:99:LYS:N	1:A:100:PRO:CD	2.82	0.42
1:C:244:TYR:CE2	1:C:254:VAL:HG11	2.52	0.42
1:B:298:VAL:HG12	1:B:299:SER:N	2.35	0.42
1:A:330:LEU:HG	1:A:331:GLU:N	2.35	0.42
1:E:370:GLN:HG2	1:E:371:LYS:O	2.20	0.42
1:F:99:LYS:N	1:F:100:PRO:CD	2.81	0.42
1:B:217:ARG:NH1	1:B:217:ARG:CB	2.83	0.42
1:D:458:GLN:HG3	1:D:459:GLU:N	2.35	0.42
1:B:217:ARG:CZ	1:B:217:ARG:HB2	2.50	0.42
1:C:224:ASP:O	1:C:226:PRO:HD3	2.20	0.42
1:E:146:ASN:HD21	1:E:148:VAL:HB	1.84	0.42
1:E:214:ASN:HD21	1:F:246:LYS:CE	2.32	0.42
1:E:293:ASN:HA	1:E:318:ILE:CD1	2.50	0.42
1:F:358:LEU:C	1:F:360:TYR:H	2.23	0.42
1:D:293:ASN:C	1:D:318:ILE:HD12	2.40	0.42
1:A:386:GLN:HG3	1:A:410:ASN:O	2.20	0.42
1:D:336:THR:O	1:D:337:LYS:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LEU:O	1:B:294:LYS:HG2	2.20	0.42
1:D:393:ASP:HA	1:D:396:LEU:HD12	2.01	0.42
1:C:246:LYS:CE	1:D:214:ASN:ND2	2.83	0.42
1:A:270:GLU:HB3	1:A:307:TYR:CD2	2.55	0.42
1:F:224:ASP:O	1:F:226:PRO:HD3	2.20	0.42
1:E:147:SER:HB3	1:E:152:TYR:CE1	2.55	0.42
1:C:142:ARG:HA	1:C:142:ARG:HD2	1.84	0.42
1:C:373:TRP:C	1:C:375:ILE:H	2.21	0.41
1:A:336:THR:O	1:A:337:LYS:C	2.58	0.41
1:C:90:ALA:HB2	1:C:169:PHE:HD1	1.85	0.41
1:C:294:LYS:HA	1:C:378:ASP:OD2	2.20	0.41
1:C:374:ASN:HA	1:C:400:ASN:ND2	2.35	0.41
1:D:362:LYS:HB3	1:D:362:LYS:HE2	1.85	0.41
1:D:217:ARG:CZ	1:D:217:ARG:HB2	2.50	0.41
1:F:400:ASN:O	1:F:401:LYS:CB	2.68	0.41
1:C:293:ASN:C	1:C:318:ILE:HD12	2.41	0.41
1:B:258:LYS:HZ1	1:B:449:ASN:ND2	2.17	0.41
1:F:297:LEU:HD22	1:F:372:PRO:HB2	2.01	0.41
1:D:117:GLU:HB3	1:F:125:ARG:HD3	2.02	0.41
1:F:60:TYR:HB3	1:F:69:GLN:NE2	2.35	0.41
1:E:224:ASP:O	1:E:226:PRO:HD3	2.21	0.41
1:E:217:ARG:CZ	1:E:217:ARG:HB2	2.51	0.41
1:F:329:ILE:HD11	1:F:354:LEU:O	2.20	0.41
1:A:326:ASN:O	1:A:366:TYR:OH	2.38	0.41
1:C:90:ALA:HB2	1:C:169:PHE:CD1	2.55	0.41
1:B:301:SER:OG	1:B:347:LYS:HE2	2.19	0.41
1:C:458:GLN:HG3	1:C:459:GLU:N	2.35	0.41
1:E:336:THR:O	1:E:337:LYS:C	2.58	0.41
1:D:498:LEU:HA	1:D:498:LEU:HD23	1.87	0.41
1:E:451:MET:HE1	1:E:455:TRP:HE1	1.84	0.41
1:B:429:CYS:HA	1:B:430:PRO:HD3	1.88	0.41
1:E:181:THR:HG22	1:E:183:LEU:HG	2.02	0.41
1:D:214:ASN:N	1:D:214:ASN:ND2	2.62	0.41
1:F:153:LYS:HD2	1:F:225:VAL:O	2.20	0.41
1:B:330:LEU:HG	1:B:331:GLU:N	2.35	0.41
1:E:78:VAL:HA	1:E:88:LEU:HD21	2.02	0.41
1:E:99:LYS:HE2	1:E:103:LYS:HE3	2.01	0.41
1:D:217:ARG:NH1	1:D:217:ARG:HB2	2.35	0.41
1:D:57:ASN:OD1	1:D:57:ASN:C	2.59	0.41
1:F:90:ALA:HB2	1:F:169:PHE:CD1	2.56	0.41
1:E:270:GLU:HB3	1:E:307:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:324:ASP:HB2	1:F:354:LEU:HD22	2.01	0.41
1:C:354:LEU:O	1:C:354:LEU:HD12	2.20	0.41
1:D:258:LYS:HZ1	1:D:449:ASN:ND2	2.17	0.41
1:C:469:LYS:O	1:C:473:GLU:HG3	2.20	0.41
1:C:498:LEU:HD23	1:C:498:LEU:HA	1.87	0.41
1:D:451:MET:HE3	1:D:453:LEU:HD12	2.03	0.41
1:B:153:LYS:HG3	1:B:185:MET:HE2	2.02	0.41
1:D:181:THR:HG22	1:D:183:LEU:HG	2.02	0.41
1:C:451:MET:CE	1:C:455:TRP:HE1	2.33	0.41
1:E:458:GLN:HG3	1:E:459:GLU:N	2.35	0.41
1:F:430:PRO:HG3	1:F:489:VAL:CA	2.43	0.41
1:F:258:LYS:HZ1	1:F:449:ASN:ND2	2.18	0.41
1:A:376:PRO:N	1:A:400:ASN:HD22	2.19	0.41
1:A:469:LYS:O	1:A:473:GLU:HG3	2.21	0.41
1:C:285:LYS:HG2	1:C:285:LYS:O	2.20	0.41
1:E:363:THR:O	1:E:363:THR:HG22	2.20	0.41
1:D:469:LYS:O	1:D:473:GLU:HG3	2.21	0.41
1:B:146:ASN:HD21	1:B:148:VAL:HB	1.85	0.41
1:D:224:ASP:O	1:D:226:PRO:HD3	2.21	0.41
1:F:483:LEU:O	1:F:484:ASN:HB3	2.20	0.41
1:B:469:LYS:O	1:B:473:GLU:HG3	2.21	0.41
1:E:297:LEU:HD22	1:E:372:PRO:HB2	2.02	0.41
1:B:159:HIS:HA	1:B:160:PRO:HD3	1.95	0.41
1:F:398:ILE:CA	1:F:426:ILE:HD11	2.51	0.41
1:B:295:LYS:N	1:B:378:ASP:OD2	2.52	0.41
1:F:376:PRO:HA	1:F:400:ASN:HB3	2.03	0.41
1:F:319:VAL:HG13	1:F:319:VAL:O	2.21	0.41
1:A:90:ALA:O	1:A:94:VAL:HG23	2.21	0.41
1:E:295:LYS:CG	1:E:320:LEU:HD11	2.51	0.40
1:F:153:LYS:HG3	1:F:185:MET:HE3	2.02	0.40
1:B:153:LYS:HD2	1:B:225:VAL:O	2.21	0.40
1:D:398:ILE:H	1:D:398:ILE:HG13	1.71	0.40
1:A:153:LYS:HG3	1:A:185:MET:HE2	2.02	0.40
1:E:468:MET:CE	1:E:471:ILE:HD12	2.51	0.40
1:E:258:LYS:HZ1	1:E:449:ASN:ND2	2.18	0.40
1:B:90:ALA:HB2	1:B:169:PHE:CD1	2.56	0.40
1:C:181:THR:HG22	1:C:183:LEU:HG	2.03	0.40
1:C:346:ILE:CD1	1:C:357:TYR:CA	2.98	0.40
1:D:128:TRP:HE1	1:D:138:ASN:ND2	2.16	0.40
1:E:293:ASN:HA	1:E:318:ILE:HD12	2.04	0.40
1:F:330:LEU:HG	1:F:331:GLU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:LYS:NZ	2:E:540:HOH:O	2.36	0.40
1:E:409:ALA:O	1:E:412:PRO:HD3	2.21	0.40
1:B:451:MET:HE1	1:B:455:TRP:HE1	1.87	0.40
1:E:90:ALA:HB2	1:E:169:PHE:CD1	2.56	0.40
1:E:359:LYS:HG2	1:E:359:LYS:O	2.20	0.40
1:F:437:GLY:O	1:F:441:VAL:HG23	2.21	0.40
1:A:137:MET:HG2	1:A:138:ASN:N	2.36	0.40
1:E:371:LYS:HD2	1:E:371:LYS:N	2.37	0.40
1:F:90:ALA:HB2	1:F:169:PHE:HD1	1.87	0.40
1:C:61:THR:HG22	1:C:61:THR:O	2.20	0.40
1:F:373:TRP:HE3	1:F:373:TRP:HA	1.87	0.40
1:F:295:LYS:HA	1:F:318:ILE:HG22	2.03	0.40
1:C:78:VAL:HA	1:C:88:LEU:HD21	2.03	0.40
1:E:154:GLY:HA3	1:E:188:GLY:O	2.22	0.40
1:E:437:GLY:O	1:E:441:VAL:HG23	2.22	0.40
1:E:356:GLU:HA	1:E:356:GLU:OE1	2.22	0.40
1:F:464:LEU:HD12	1:F:464:LEU:O	2.21	0.40
1:F:354:LEU:C	1:F:356:GLU:N	2.75	0.40
1:C:153:LYS:HG3	1:C:185:MET:HE3	2.02	0.40
1:B:62:SER:C	1:B:64:LYS:H	2.25	0.40
1:B:418:LEU:HD23	1:B:418:LEU:C	2.41	0.40
1:E:418:LEU:HD23	1:E:418:LEU:C	2.42	0.40
1:E:217:ARG:NH1	1:E:217:ARG:CB	2.84	0.40
1:B:451:MET:HE3	1:B:453:LEU:HD12	2.03	0.40
1:B:393:ASP:HA	1:B:396:LEU:HD12	2.03	0.40
1:F:146:ASN:HD21	1:F:148:VAL:HB	1.86	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	454/456 (100%)	407 (90%)	39 (9%)	8 (2%)	11	42
1	B	454/456 (100%)	403 (89%)	44 (10%)	7 (2%)	13	46
1	C	454/456 (100%)	398 (88%)	48 (11%)	8 (2%)	11	42
1	D	454/456 (100%)	414 (91%)	37 (8%)	3 (1%)	26	65
1	E	454/456 (100%)	391 (86%)	52 (12%)	11 (2%)	7	33
1	F	454/456 (100%)	404 (89%)	45 (10%)	5 (1%)	17	55
All	All	2724/2736 (100%)	2417 (89%)	265 (10%)	42 (2%)	13	46

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
1	E	62	SER
1	A	66	VAL
1	A	267	ILE
1	A	318	ILE
1	B	59	GLY
1	B	267	ILE
1	B	318	ILE
1	C	267	ILE
1	C	318	ILE
1	C	369	ASN
1	D	267	ILE
1	D	318	ILE
1	E	64	LYS
1	E	267	ILE
1	E	318	ILE
1	E	363	THR
1	E	387	ASN
1	F	267	ILE
1	F	318	ILE
1	F	373	TRP
1	A	271	ALA
1	A	350	GLN
1	B	61	THR
1	B	64	LYS
1	B	358	LEU
1	C	351	ARG
1	E	271	ALA
1	E	353	ARG
1	E	401	LYS

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Mol	Chain	Res	Type
1	A	349	ASN
1	A	351	ARG
1	B	271	ALA
1	C	271	ALA
1	C	356	GLU
1	C	374	ASN
1	D	271	ALA
1	E	366	TYR
1	F	271	ALA
1	F	387	ASN
1	C	368	GLU
1	E	384	ALA

### 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	393/393 (100%)	386 (98%)	7 (2%)	66	88
1	B	393/393 (100%)	383 (98%)	10 (2%)	55	84
1	C	393/393 (100%)	384 (98%)	9 (2%)	58	84
1	D	393/393 (100%)	382 (97%)	11 (3%)	51	82
1	E	393/393 (100%)	385 (98%)	8 (2%)	63	86
1	F	393/393 (100%)	384 (98%)	9 (2%)	58	84
All	All	2358/2358 (100%)	2304 (98%)	54 (2%)	58	84

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	TYR
1	A	169	PHE
1	A	214	ASN
1	A	216	PHE
1	A	286	ASP
1	A	390	ASN

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Mol	Chain	Res	Type
1	A	399	GLN
1	B	56	HIS
1	B	60	TYR
1	B	145	TYR
1	B	169	PHE
1	B	214	ASN
1	B	216	PHE
1	B	286	ASP
1	B	297	LEU
1	B	351	ARG
1	B	360	TYR
1	C	145	TYR
1	C	169	PHE
1	C	214	ASN
1	C	216	PHE
1	C	286	ASP
1	C	355	LYS
1	C	363	THR
1	C	374	ASN
1	C	401	LYS
1	D	145	TYR
1	D	169	PHE
1	D	214	ASN
1	D	216	PHE
1	D	286	ASP
1	D	298	VAL
1	D	353	ARG
1	D	363	THR
1	D	368	GLU
1	D	386	GLN
1	D	393	ASP
1	E	60	TYR
1	E	145	TYR
1	E	169	PHE
1	E	214	ASN
1	E	216	PHE
1	E	286	ASP
1	E	374	ASN
1	E	378	ASP
1	F	56	HIS
1	F	145	TYR
1	F	169	PHE

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Mol	Chain	Res	Type
1	F	214	ASN
1	F	216	PHE
1	F	286	ASP
1	F	351	ARG
1	F	352	LEU
1	F	393	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	138	ASN
1	A	146	ASN
1	A	159	HIS
1	A	214	ASN
1	A	259	ASN
1	A	290	ASN
1	A	303	ASN
1	A	339	GLN
1	A	390	ASN
1	A	400	ASN
1	A	449	ASN
1	B	56	HIS
1	B	68	ASN
1	B	138	ASN
1	B	146	ASN
1	B	159	HIS
1	B	214	ASN
1	B	259	ASN
1	B	290	ASN
1	B	350	GLN
1	B	370	GLN
1	B	390	ASN
1	B	392	ASN
1	B	449	ASN
1	C	68	ASN
1	C	138	ASN
1	C	146	ASN
1	C	159	HIS
1	C	214	ASN
1	C	259	ASN
1	C	290	ASN

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Mol	Chain	Res	Type
1	C	339	GLN
1	C	392	ASN
1	C	449	ASN
1	D	68	ASN
1	D	138	ASN
1	D	146	ASN
1	D	159	HIS
1	D	214	ASN
1	D	259	ASN
1	D	290	ASN
1	D	303	ASN
1	D	339	GLN
1	D	348	ASN
1	D	386	GLN
1	D	390	ASN
1	D	399	GLN
1	D	449	ASN
1	E	57	ASN
1	E	69	GLN
1	E	138	ASN
1	E	146	ASN
1	E	159	HIS
1	E	214	ASN
1	E	259	ASN
1	E	290	ASN
1	E	326	ASN
1	E	370	GLN
1	E	374	ASN
1	E	400	ASN
1	E	449	ASN
1	F	69	GLN
1	F	138	ASN
1	F	146	ASN
1	F	159	HIS
1	F	214	ASN
1	F	259	ASN
1	F	290	ASN
1	F	339	GLN
1	F	370	GLN
1	F	392	ASN
1	F	399	GLN
1	F	449	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 carbohydrates 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	456/456 (100%)	-0.03	2 (0%) 93 85	43, 66, 101, 121	0
1	B	456/456 (100%)	0.08	6 (1%) 79 62	42, 68, 108, 121	0
1	C	456/456 (100%)	0.18	20 (4%) 38 17	42, 68, 113, 137	0
1	D	456/456 (100%)	0.00	1 (0%) 95 91	43, 65, 104, 120	0
1	E	456/456 (100%)	0.22	31 (6%) 20 7	42, 69, 124, 133	0
1	F	456/456 (100%)	-0.01	1 (0%) 95 91	42, 66, 98, 121	0
All	All	2736/2736 (100%)	0.07	61 (2%) 65 42	42, 67, 111, 137	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	361	SER	3.7
1	E	333	ASN	3.7
1	C	428	LEU	3.5
1	E	365	LYS	3.4
1	E	343	ILE	3.2
1	C	419	HIS	3.2
1	C	342	TYR	3.2
1	E	300	GLY	3.2
1	E	288	ASN	3.1
1	C	423	GLN	3.1
1	E	354	LEU	3.0
1	E	322	MET	2.9
1	B	55	LEU	2.9
1	C	70	ILE	2.8
1	B	346	ILE	2.8
1	E	413	THR	2.8
1	B	333	ASN	2.7
1	C	61	THR	2.7
1	E	392	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	359	LYS	2.6
1	C	343	ILE	2.6
1	C	62	SER	2.6
1	B	62	SER	2.6
1	E	356	GLU	2.6
1	E	387	ASN	2.5
1	E	330	LEU	2.5
1	C	429	CYS	2.5
1	C	360	TYR	2.5
1	C	420	LYS	2.5
1	A	353	ARG	2.4
1	E	355	LYS	2.4
1	E	484	ASN	2.4
1	B	345	ASP	2.4
1	C	458	GLN	2.4
1	C	390	ASN	2.3
1	E	353	ARG	2.3
1	C	422	LYS	2.3
1	E	342	TYR	2.3
1	E	334	GLY	2.3
1	E	372	PRO	2.3
1	C	349	ASN	2.3
1	E	370	GLN	2.3
1	C	332	PRO	2.2
1	E	414	HIS	2.2
1	C	416	LYS	2.2
1	B	413	THR	2.2
1	E	360	TYR	2.2
1	E	361	SER	2.1
1	E	423	GLN	2.1
1	D	416	LYS	2.1
1	E	301	SER	2.1
1	E	337	LYS	2.1
1	E	335	PHE	2.1
1	A	484	ASN	2.1
1	F	485	GLU	2.1
1	C	340	LEU	2.1
1	E	340	LEU	2.1
1	C	391	GLU	2.1
1	E	357	TYR	2.1
1	E	55	LEU	2.0
1	E	386	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.