



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:58 PM GMT

PDB ID : 2NVV  
Title : Crystal Structure of the Putative Acetyl-CoA hydrolase/transferasePG1013 from Porphyromonas gingivalis, Northeast Structural Genomics Target PgR16.  
Authors : Forouhar, F.; Neely, H.; Seetharaman, J.; Yong, W.; Ho, C.K.; Fang, Y.; Cunningham, K.; Ma, L.-C.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2006-11-13  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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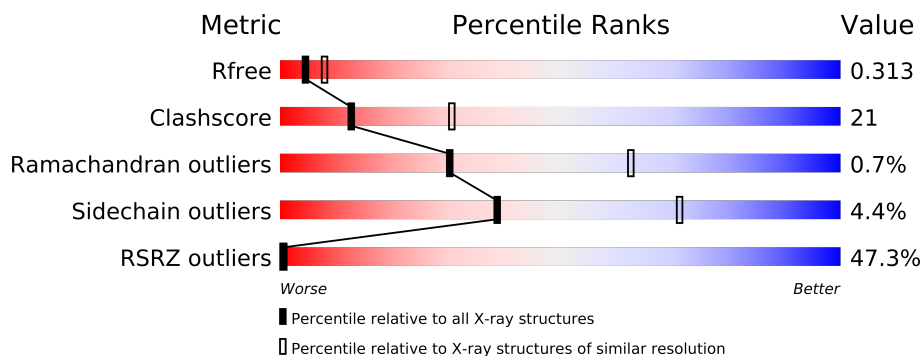
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	506	
1	B	506	
1	C	506	
1	D	506	
1	E	506	
1	F	506	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23178 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acetyl-CoA hydrolase/transferasefamily protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	B	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	C	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	D	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	E	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	F	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	57	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	168	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	170	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	243	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	281	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	294	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	372	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	373	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	397	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	408	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	488	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	497	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	499	LEU	-	EXPRESSION TAG	UNP Q7MVN7
A	500	GLU	-	EXPRESSION TAG	UNP Q7MVN7
A	501	HIS	-	EXPRESSION TAG	UNP Q7MVN7
A	502	HIS	-	EXPRESSION TAG	UNP Q7MVN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	503	HIS	-	EXPRESSION TAG	UNP Q7MVN7
A	504	HIS	-	EXPRESSION TAG	UNP Q7MVN7
A	505	HIS	-	EXPRESSION TAG	UNP Q7MVN7
A	506	HIS	-	EXPRESSION TAG	UNP Q7MVN7
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	57	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	168	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	170	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	243	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	281	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	294	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	372	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	373	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	397	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	408	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	488	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	497	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	499	LEU	-	EXPRESSION TAG	UNP Q7MVN7
B	500	GLU	-	EXPRESSION TAG	UNP Q7MVN7
B	501	HIS	-	EXPRESSION TAG	UNP Q7MVN7
B	502	HIS	-	EXPRESSION TAG	UNP Q7MVN7
B	503	HIS	-	EXPRESSION TAG	UNP Q7MVN7
B	504	HIS	-	EXPRESSION TAG	UNP Q7MVN7
B	505	HIS	-	EXPRESSION TAG	UNP Q7MVN7
B	506	HIS	-	EXPRESSION TAG	UNP Q7MVN7
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	57	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	168	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	170	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	243	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	281	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	294	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	372	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	373	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	397	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	408	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	488	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	497	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	499	LEU	-	EXPRESSION TAG	UNP Q7MVN7
C	500	GLU	-	EXPRESSION TAG	UNP Q7MVN7
C	501	HIS	-	EXPRESSION TAG	UNP Q7MVN7
C	502	HIS	-	EXPRESSION TAG	UNP Q7MVN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	503	HIS	-	EXPRESSION TAG	UNP Q7MVN7
C	504	HIS	-	EXPRESSION TAG	UNP Q7MVN7
C	505	HIS	-	EXPRESSION TAG	UNP Q7MVN7
C	506	HIS	-	EXPRESSION TAG	UNP Q7MVN7
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	57	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	168	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	170	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	243	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	281	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	294	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	372	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	373	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	397	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	408	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	488	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	497	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	499	LEU	-	EXPRESSION TAG	UNP Q7MVN7
D	500	GLU	-	EXPRESSION TAG	UNP Q7MVN7
D	501	HIS	-	EXPRESSION TAG	UNP Q7MVN7
D	502	HIS	-	EXPRESSION TAG	UNP Q7MVN7
D	503	HIS	-	EXPRESSION TAG	UNP Q7MVN7
D	504	HIS	-	EXPRESSION TAG	UNP Q7MVN7
D	505	HIS	-	EXPRESSION TAG	UNP Q7MVN7
D	506	HIS	-	EXPRESSION TAG	UNP Q7MVN7
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	57	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	168	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	170	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	243	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	281	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	294	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	372	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	373	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	397	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	408	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	488	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	497	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	499	LEU	-	EXPRESSION TAG	UNP Q7MVN7
E	500	GLU	-	EXPRESSION TAG	UNP Q7MVN7
E	501	HIS	-	EXPRESSION TAG	UNP Q7MVN7
E	502	HIS	-	EXPRESSION TAG	UNP Q7MVN7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	503	HIS	-	EXPRESSION TAG	UNP Q7MVN7
E	504	HIS	-	EXPRESSION TAG	UNP Q7MVN7
E	505	HIS	-	EXPRESSION TAG	UNP Q7MVN7
E	506	HIS	-	EXPRESSION TAG	UNP Q7MVN7
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	57	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	168	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	170	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	243	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	281	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	294	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	372	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	373	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	397	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	408	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	488	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	497	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	499	LEU	-	EXPRESSION TAG	UNP Q7MVN7
F	500	GLU	-	EXPRESSION TAG	UNP Q7MVN7
F	501	HIS	-	EXPRESSION TAG	UNP Q7MVN7
F	502	HIS	-	EXPRESSION TAG	UNP Q7MVN7
F	503	HIS	-	EXPRESSION TAG	UNP Q7MVN7
F	504	HIS	-	EXPRESSION TAG	UNP Q7MVN7
F	505	HIS	-	EXPRESSION TAG	UNP Q7MVN7
F	506	HIS	-	EXPRESSION TAG	UNP Q7MVN7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	E	2	Total Zn 2 2	0	0

- Molecule 3 is water.

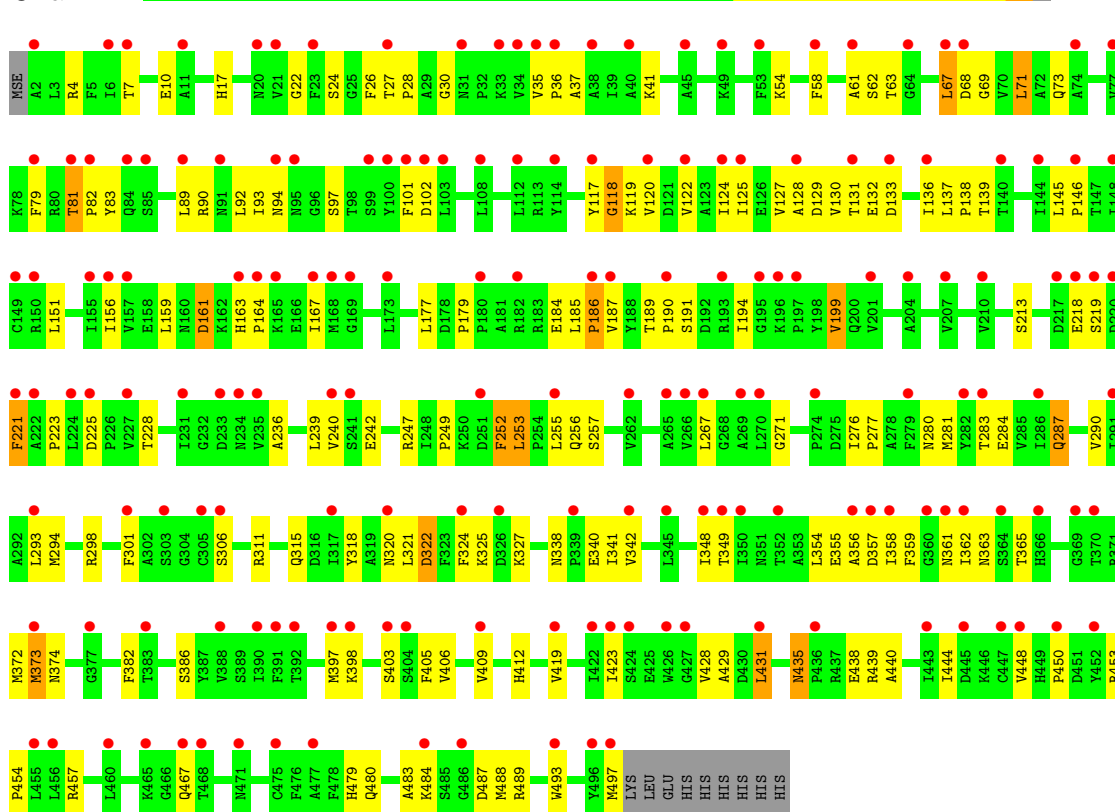
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	B	22	Total 22	O 22	0	0
3	C	30	Total 30	O 30	0	0
3	D	23	Total 23	O 23	0	0
3	E	52	Total 52	O 52	0	0
3	F	47	Total 47	O 47	0	0

### 3 Residue-property plots

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

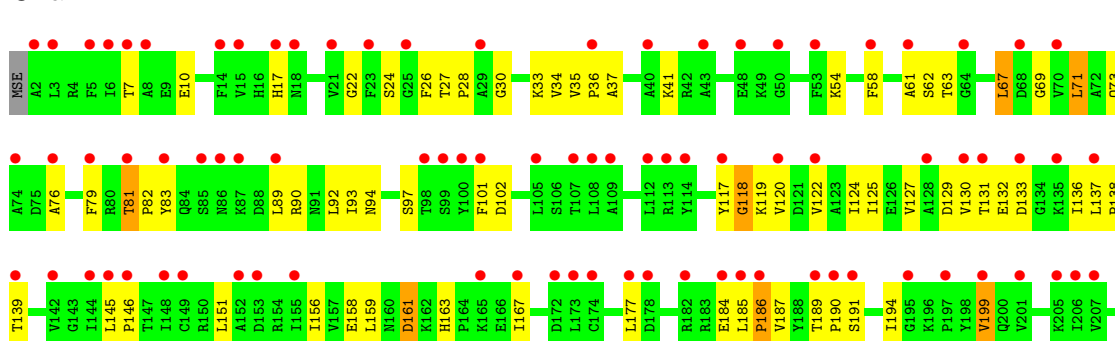
- Molecule 1: Acetyl-CoA hydrolase/transferasefamily protein

Chain A:

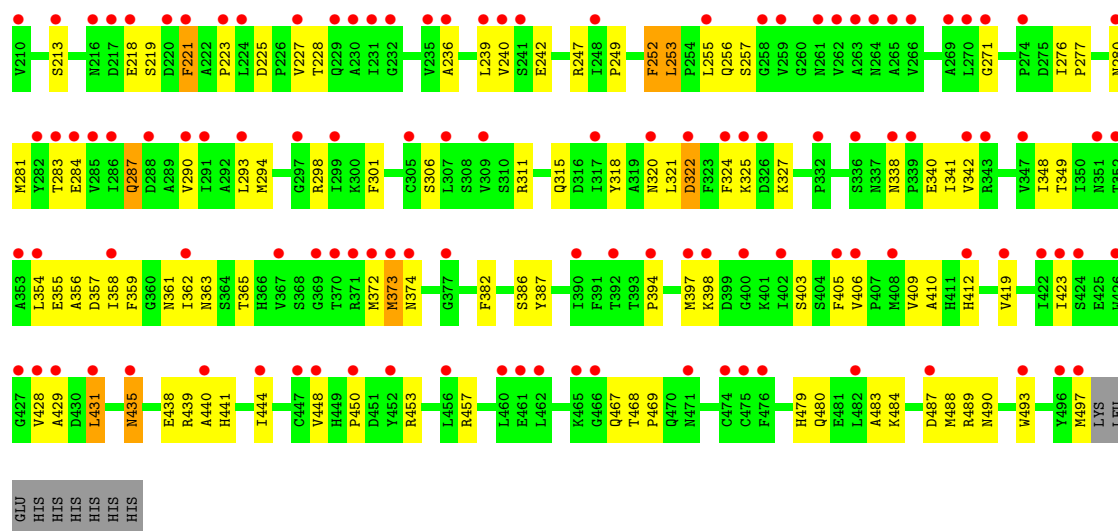


- Molecule 1: Acetyl-CoA hydrolase/transferasefamily protein

Chain B:

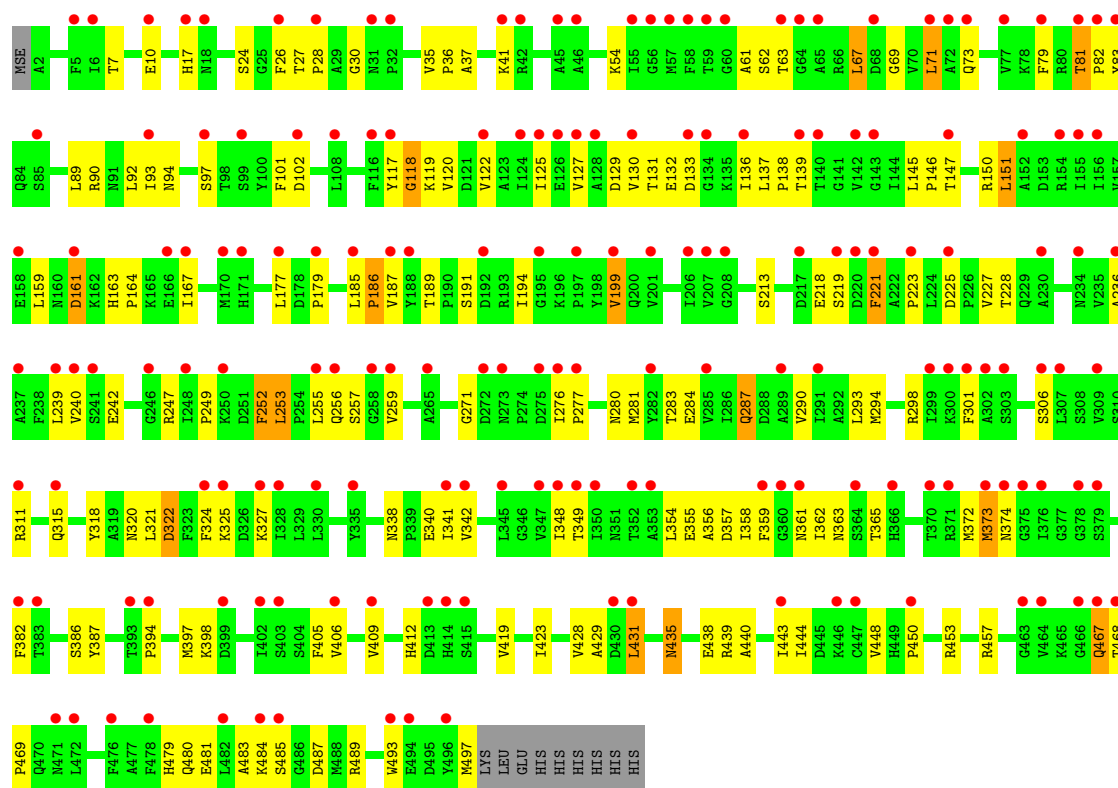






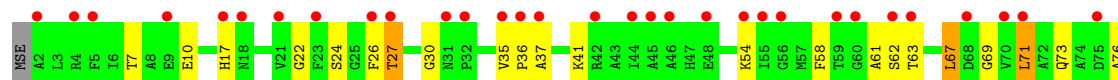
• Molecule 1: Acetyl-CoA hydrolase/transferasefamily protein

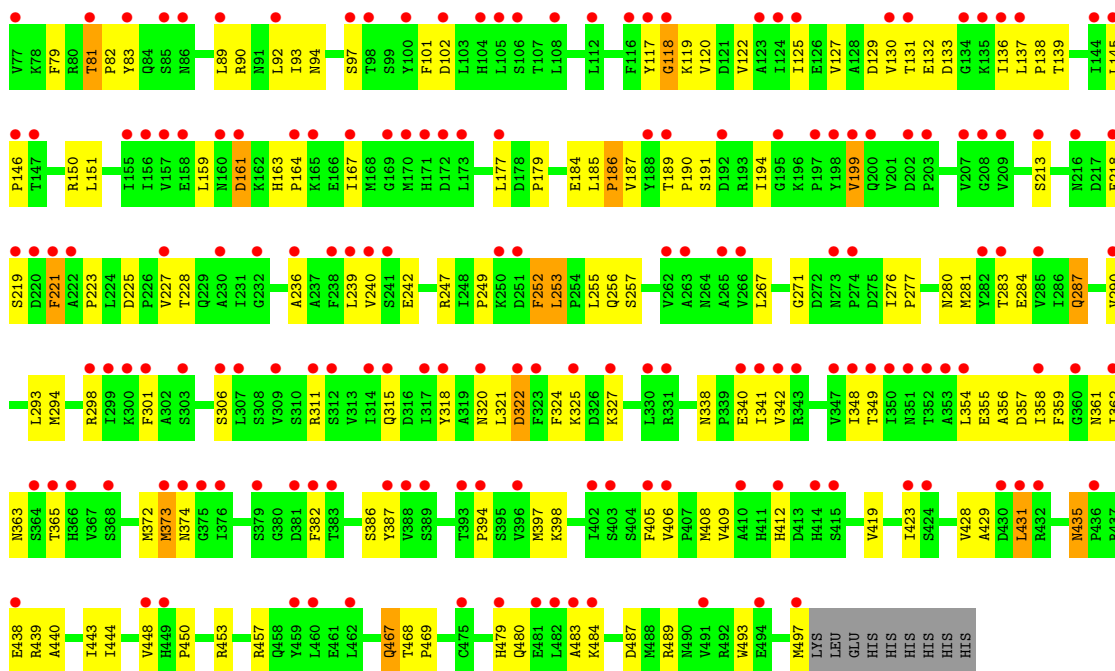
Chain C:



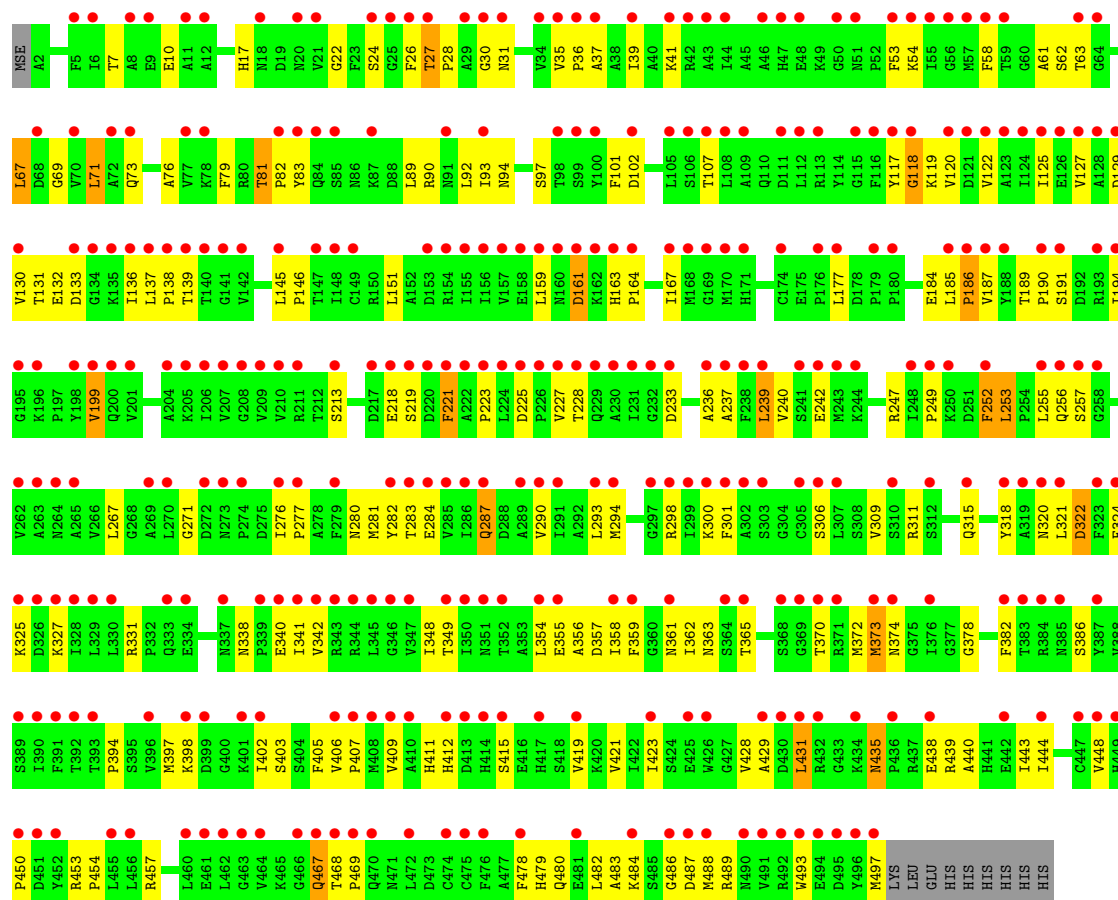
• Molecule 1: Acetyl-CoA hydrolase/transferasefamily protein

Chain D:





Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.05Å 131.05Å 162.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.70 29.46 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.95-2.70) 52.4 (29.46-2.40)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.63 (at 2.39Å)	Xtriage
Refinement program	XTALVIEW, CNS 1.1	Depositor
R, $R_{free}$	0.287 , 0.290 0.322 , 0.313	Depositor DCC
$R_{free}$ test set	4447 reflections (7.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.0	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , -5.1	EDS
Estimated twinning fraction	0.012 for H, K, L 0.496 for -H, H+K, -L 0.492 for -H, -K, L 0.025 for -h,-k,l 0.499 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.012 for H, K, L 0.496 for -H, H+K, -L 0.492 for -H, -K, L	Depositor
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 121779 reflections	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	23178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0/3898	0.66	0/5269
1	B	0.38	0/3898	0.66	0/5269
1	C	0.38	0/3898	0.66	0/5269
1	D	0.38	0/3898	0.66	0/5269
1	E	0.40	0/3898	0.65	0/5269
1	F	0.40	0/3898	0.66	0/5269
All	All	0.39	0/23388	0.66	0/31614

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3828	0	3808	155	0
1	B	3828	0	3808	154	0
1	C	3828	0	3808	150	0
1	D	3828	0	3808	154	0
1	E	3828	0	3808	173	0
1	F	3828	0	3808	191	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
3	A	30	0	0	10	0
3	B	22	0	0	9	0
3	C	30	0	0	2	0
3	D	23	0	0	2	0
3	E	52	0	0	20	0
3	F	47	0	0	30	0
All	All	23178	0	22848	957	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (957) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:298:ARG:HB2	3:A:516:HOH:O	1.58	1.03
1:F:419:VAL:HG12	3:F:517:HOH:O	1.67	0.94
1:E:136:ILE:HB	1:E:199:VAL:HG13	1.50	0.93
1:F:136:ILE:HB	1:F:199:VAL:HG13	1.51	0.92
1:A:94:ASN:HD21	1:A:372:MSE:H	1.18	0.91
1:C:94:ASN:HD21	1:C:372:MSE:H	1.18	0.91
1:C:136:ILE:HB	1:C:199:VAL:HG13	1.51	0.89
1:D:136:ILE:HB	1:D:199:VAL:HG13	1.53	0.88
1:D:94:ASN:HD21	1:D:372:MSE:H	1.21	0.88
1:B:94:ASN:HD21	1:B:372:MSE:H	1.22	0.88
1:F:94:ASN:HD21	1:F:372:MSE:H	1.22	0.88
1:A:136:ILE:HB	1:A:199:VAL:HG13	1.52	0.88
1:E:365:THR:O	1:E:373:MSE:HB2	1.75	0.87
1:D:365:THR:O	1:D:373:MSE:HB2	1.74	0.87
1:E:94:ASN:HD21	1:E:372:MSE:H	1.21	0.87
1:B:136:ILE:HB	1:B:199:VAL:HG13	1.53	0.87
1:F:365:THR:O	1:F:373:MSE:HB2	1.74	0.86
1:F:127:VAL:HG12	1:F:129:ASP:H	1.42	0.85
1:A:340:GLU:HG3	1:B:340:GLU:HG3	1.58	0.85
1:A:127:VAL:HG12	1:A:129:ASP:H	1.42	0.84
1:F:17:HIS:HD2	1:F:54:LYS:H	1.25	0.84
1:B:36:PRO:HD2	3:B:513:HOH:O	1.75	0.84
1:E:447:CYS:HB2	3:E:541:HOH:O	1.77	0.84
1:C:365:THR:O	1:C:373:MSE:HB2	1.78	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:17:HIS:HD2	1:B:54:LYS:H	1.26	0.84
1:A:365:THR:O	1:A:373:MSE:HB2	1.78	0.83
1:E:127:VAL:HG12	1:E:129:ASP:H	1.43	0.83
1:B:365:THR:O	1:B:373:MSE:HB2	1.77	0.83
1:B:127:VAL:HG12	1:B:129:ASP:H	1.44	0.83
1:D:17:HIS:HD2	1:D:54:LYS:H	1.26	0.83
1:A:17:HIS:HD2	1:A:54:LYS:H	1.25	0.83
1:C:127:VAL:HG12	1:C:129:ASP:H	1.44	0.82
1:C:17:HIS:HD2	1:C:54:LYS:H	1.27	0.82
1:A:480:GLN:O	1:A:484:LYS:HG2	1.79	0.82
1:E:17:HIS:HD2	1:E:54:LYS:H	1.23	0.82
1:E:256:GLN:HA	1:E:283:THR:CG2	2.10	0.81
1:D:480:GLN:O	1:D:484:LYS:HG2	1.81	0.81
1:C:480:GLN:O	1:C:484:LYS:HG2	1.79	0.80
1:D:127:VAL:HG12	1:D:129:ASP:H	1.46	0.80
1:B:256:GLN:HA	1:B:283:THR:CG2	2.11	0.80
1:A:256:GLN:HA	1:A:283:THR:CG2	2.12	0.80
1:D:81:THR:HG22	1:D:82:PRO:HA	1.64	0.80
1:C:256:GLN:HA	1:C:283:THR:CG2	2.13	0.79
1:E:450:PRO:HA	1:E:453:ARG:HG3	1.62	0.79
1:F:81:THR:HG22	1:F:82:PRO:HA	1.65	0.79
1:F:187:VAL:HG21	3:F:527:HOH:O	1.82	0.79
1:C:450:PRO:HA	1:C:453:ARG:HG3	1.64	0.79
1:B:480:GLN:O	1:B:484:LYS:HG2	1.81	0.78
1:B:450:PRO:HA	1:B:453:ARG:HG3	1.65	0.78
1:D:256:GLN:HA	1:D:283:THR:CG2	2.13	0.78
1:E:480:GLN:O	1:E:484:LYS:HG2	1.82	0.78
1:A:450:PRO:HA	1:A:453:ARG:HG3	1.65	0.78
1:A:81:THR:HG22	1:A:82:PRO:HA	1.65	0.78
1:B:81:THR:HG22	1:B:82:PRO:HA	1.66	0.78
1:F:450:PRO:HA	1:F:453:ARG:HG3	1.65	0.78
1:C:81:THR:HG22	1:C:82:PRO:HA	1.65	0.78
1:F:370:THR:HG23	3:F:550:HOH:O	1.85	0.77
1:F:480:GLN:O	1:F:484:LYS:HG2	1.83	0.77
1:E:435:ASN:HD21	1:E:438:GLU:HG3	1.50	0.77
1:C:340:GLU:HG3	1:D:340:GLU:HG3	1.66	0.77
1:C:493:TRP:O	1:C:497:MSE:HG2	1.85	0.76
1:A:127:VAL:HG12	1:A:129:ASP:N	1.99	0.76
1:E:340:GLU:HG3	1:F:340:GLU:HG3	1.67	0.76
1:E:81:THR:HG22	1:E:82:PRO:HA	1.68	0.76
1:E:293:LEU:HD22	1:E:298:ARG:HG2	1.67	0.76
1:E:493:TRP:O	1:E:497:MSE:HG2	1.86	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:294:MSE:HE3	1:D:327:LYS:HB2	1.66	0.76
1:B:127:VAL:HG12	1:B:129:ASP:N	2.01	0.76
1:F:127:VAL:HG12	1:F:129:ASP:N	2.01	0.76
1:A:256:GLN:HA	1:A:283:THR:HG22	1.68	0.76
1:C:127:VAL:HG12	1:C:129:ASP:N	2.01	0.76
3:E:525:HOH:O	1:F:107:THR:HA	1.85	0.76
1:A:493:TRP:O	1:A:497:MSE:HG2	1.86	0.76
1:F:431:LEU:HD22	3:F:517:HOH:O	1.85	0.75
1:F:493:TRP:O	1:F:497:MSE:HG2	1.85	0.75
1:E:256:GLN:HA	1:E:283:THR:HG22	1.69	0.75
1:B:294:MSE:HE3	1:B:327:LYS:HB2	1.68	0.75
1:E:127:VAL:HG12	1:E:129:ASP:N	2.01	0.75
1:C:294:MSE:HE3	1:C:327:LYS:HB2	1.67	0.75
1:D:293:LEU:HD22	1:D:298:ARG:HG2	1.68	0.75
1:B:256:GLN:HA	1:B:283:THR:HG22	1.69	0.75
1:F:256:GLN:HA	1:F:283:THR:CG2	2.15	0.74
1:F:294:MSE:HE3	1:F:327:LYS:HB2	1.67	0.74
1:F:293:LEU:HD22	1:F:298:ARG:HG2	1.69	0.74
1:F:321:LEU:HD21	3:F:544:HOH:O	1.86	0.74
1:B:493:TRP:O	1:B:497:MSE:HG2	1.87	0.74
1:A:294:MSE:HE3	1:A:327:LYS:HB2	1.68	0.74
1:F:435:ASN:HD21	1:F:438:GLU:HG3	1.52	0.74
1:A:293:LEU:HD22	1:A:298:ARG:HG2	1.68	0.74
1:D:450:PRO:HA	1:D:453:ARG:HG3	1.68	0.74
1:D:493:TRP:O	1:D:497:MSE:HG2	1.88	0.74
1:C:256:GLN:HA	1:C:283:THR:HG22	1.70	0.73
1:D:256:GLN:HA	1:D:283:THR:HG22	1.70	0.73
1:E:24:SER:HB3	1:E:125:ILE:HG22	1.69	0.73
1:D:127:VAL:HG12	1:D:129:ASP:N	2.02	0.73
1:E:444:ILE:O	1:E:453:ARG:HD2	1.88	0.73
1:B:293:LEU:HD22	1:B:298:ARG:HG2	1.71	0.72
1:E:447:CYS:HA	3:E:515:HOH:O	1.90	0.71
1:D:435:ASN:ND2	1:D:438:GLU:H	1.88	0.71
1:C:293:LEU:HD22	1:C:298:ARG:HG2	1.72	0.71
1:E:106:SER:HB2	3:E:554:HOH:O	1.91	0.71
1:B:435:ASN:HD21	1:B:438:GLU:HG3	1.54	0.71
1:C:444:ILE:O	1:C:453:ARG:HD2	1.90	0.71
1:F:256:GLN:HA	1:F:283:THR:HG22	1.73	0.71
3:E:545:HOH:O	1:F:415:SER:HB2	1.91	0.71
1:D:435:ASN:HD21	1:D:438:GLU:HG3	1.56	0.70
1:B:479:HIS:NE2	3:B:524:HOH:O	2.23	0.70
1:E:294:MSE:HE3	1:E:327:LYS:HB2	1.72	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:444:ILE:O	1:B:453:ARG:HD2	1.92	0.70
1:F:482:LEU:O	3:F:531:HOH:O	2.07	0.70
1:A:117:TYR:O	3:A:513:HOH:O	2.08	0.70
1:F:444:ILE:O	1:F:453:ARG:HD2	1.91	0.70
1:A:435:ASN:ND2	1:A:438:GLU:H	1.90	0.69
1:D:444:ILE:O	1:D:453:ARG:HD2	1.91	0.69
1:C:435:ASN:ND2	1:C:438:GLU:H	1.90	0.69
1:E:36:PRO:HG2	3:E:546:HOH:O	1.90	0.69
1:D:24:SER:HB3	1:D:125:ILE:HG22	1.74	0.69
1:C:435:ASN:HD21	1:C:438:GLU:HG3	1.58	0.68
1:A:444:ILE:O	1:A:453:ARG:HD2	1.92	0.68
1:F:435:ASN:ND2	1:F:438:GLU:H	1.92	0.68
1:B:435:ASN:ND2	1:B:438:GLU:H	1.90	0.68
1:C:7:THR:OG1	1:C:10:GLU:HG3	1.93	0.68
1:A:24:SER:HB3	1:A:125:ILE:HG22	1.75	0.68
1:D:7:THR:OG1	1:D:10:GLU:HG3	1.93	0.68
1:E:299:ILE:HG22	3:E:556:HOH:O	1.92	0.68
1:C:81:THR:HG23	1:C:101:PHE:O	1.94	0.68
1:E:338:ASN:HB3	1:E:341:ILE:HG12	1.76	0.67
1:A:340:GLU:CG	1:B:340:GLU:HG3	2.24	0.67
1:C:349:THR:HG21	1:C:382:PHE:HB3	1.75	0.67
1:D:349:THR:HG21	1:D:382:PHE:HB3	1.76	0.67
1:A:435:ASN:HD21	1:A:438:GLU:HG3	1.58	0.67
1:E:294:MSE:HE2	1:E:324:PHE:CD2	2.30	0.67
1:F:478:PHE:HB2	3:F:538:HOH:O	1.92	0.67
1:A:340:GLU:HG3	1:B:340:GLU:CG	2.24	0.67
1:F:349:THR:HG21	1:F:382:PHE:HB3	1.76	0.67
1:F:164:PRO:HG2	3:F:544:HOH:O	1.93	0.67
1:B:349:THR:HG21	1:B:382:PHE:HB3	1.77	0.67
1:E:349:THR:HG21	1:E:382:PHE:HB3	1.75	0.67
1:B:7:THR:OG1	1:B:10:GLU:HG3	1.94	0.67
1:E:355:GLU:HG2	1:E:363:ASN:HB3	1.77	0.67
1:C:294:MSE:HE3	1:C:327:LYS:CB	2.25	0.66
1:A:187:VAL:HG13	1:A:341:ILE:HD12	1.78	0.66
1:E:435:ASN:ND2	1:E:438:GLU:H	1.92	0.66
1:C:187:VAL:HG13	1:C:341:ILE:HD12	1.76	0.66
1:F:338:ASN:HB3	1:F:341:ILE:HG12	1.76	0.66
1:A:349:THR:HG21	1:A:382:PHE:HB3	1.77	0.66
1:F:7:THR:OG1	1:F:10:GLU:HG3	1.94	0.66
1:D:187:VAL:HG13	1:D:341:ILE:HD12	1.77	0.66
1:A:338:ASN:HB3	1:A:341:ILE:HG12	1.78	0.66
1:B:81:THR:HG23	1:B:101:PHE:O	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:26:PHE:HB3	1:E:306:SER:HB3	1.78	0.65
1:E:163:HIS:HD2	1:E:318:TYR:OH	1.79	0.65
1:C:187:VAL:CG1	1:C:341:ILE:HD12	2.27	0.65
1:D:163:HIS:HD2	1:D:318:TYR:OH	1.78	0.65
1:E:187:VAL:HG13	1:E:341:ILE:HD12	1.79	0.65
1:F:127:VAL:CG1	1:F:129:ASP:H	2.10	0.65
1:F:282:TYR:HE1	3:F:527:HOH:O	1.79	0.65
1:C:24:SER:HB3	1:C:125:ILE:HG22	1.76	0.65
1:F:81:THR:HG23	1:F:101:PHE:O	1.96	0.65
1:D:81:THR:HG23	1:D:101:PHE:O	1.97	0.65
1:F:294:MSE:HE3	1:F:327:LYS:CB	2.26	0.65
1:F:190:PRO:HB2	3:F:545:HOH:O	1.96	0.65
1:E:256:GLN:HA	1:E:283:THR:HG23	1.78	0.64
1:A:81:THR:HG23	1:A:101:PHE:O	1.97	0.64
1:B:483:ALA:HB3	1:B:484:LYS:HE3	1.78	0.64
1:E:7:THR:OG1	1:E:10:GLU:HG3	1.97	0.64
1:B:187:VAL:HG13	1:B:341:ILE:HD12	1.79	0.64
1:D:311:ARG:O	1:D:315:GLN:HG3	1.97	0.64
1:B:412:HIS:HD2	3:B:512:HOH:O	1.80	0.64
1:A:163:HIS:HD2	1:A:318:TYR:OH	1.79	0.64
1:D:294:MSE:HE3	1:D:327:LYS:CB	2.27	0.64
1:C:435:ASN:HD21	1:C:438:GLU:H	1.44	0.64
1:B:338:ASN:HB3	1:B:341:ILE:HG12	1.78	0.64
1:A:127:VAL:CG1	1:A:129:ASP:H	2.10	0.64
1:F:294:MSE:HE2	1:F:324:PHE:CD2	2.33	0.64
1:F:163:HIS:HD2	1:F:318:TYR:OH	1.79	0.64
1:C:338:ASN:HB3	1:C:341:ILE:HG12	1.79	0.64
1:D:338:ASN:HB3	1:D:341:ILE:HG12	1.80	0.64
1:D:435:ASN:HD21	1:D:438:GLU:H	1.46	0.64
1:A:184:GLU:HG3	1:B:184:GLU:HG3	1.80	0.64
1:F:355:GLU:HG2	1:F:363:ASN:HB3	1.78	0.64
1:D:355:GLU:HG2	1:D:363:ASN:HB3	1.79	0.64
1:A:294:MSE:HE2	1:A:324:PHE:CD2	2.33	0.63
1:B:163:HIS:HD2	1:B:318:TYR:OH	1.80	0.63
1:C:127:VAL:CG1	1:C:129:ASP:H	2.12	0.63
1:F:167:ILE:HD11	1:F:318:TYR:CE2	2.33	0.63
1:A:26:PHE:HB3	1:A:306:SER:HB3	1.80	0.63
1:D:294:MSE:HE2	1:D:324:PHE:CD2	2.34	0.63
1:B:355:GLU:HG2	1:B:363:ASN:HB3	1.78	0.63
1:E:127:VAL:CG1	1:E:129:ASP:H	2.12	0.63
1:A:483:ALA:HB3	1:A:484:LYS:HE3	1.80	0.63
1:B:26:PHE:HB3	1:B:306:SER:HB3	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:26:PHE:HB3	1:C:306:SER:HB3	1.80	0.63
1:B:287:GLN:HE21	1:B:287:GLN:H	1.46	0.63
1:B:294:MSE:HE3	1:B:327:LYS:CB	2.28	0.63
1:E:187:VAL:CG1	1:E:341:ILE:HD12	2.29	0.63
1:E:189:THR:HG22	1:E:191:SER:H	1.64	0.63
1:F:119:LYS:HG2	1:F:120:VAL:N	2.14	0.63
1:B:24:SER:HB3	1:B:125:ILE:HG22	1.79	0.63
1:A:7:THR:OG1	1:A:10:GLU:HG3	1.98	0.63
1:A:94:ASN:HD21	1:A:372:MSE:N	1.94	0.62
1:C:355:GLU:HG2	1:C:363:ASN:HB3	1.80	0.62
1:E:81:THR:HG23	1:E:101:PHE:O	1.99	0.62
1:A:294:MSE:HE3	1:A:327:LYS:CB	2.29	0.62
1:A:355:GLU:HG2	1:A:363:ASN:HB3	1.81	0.62
1:F:457:ARG:NH2	3:F:515:HOH:O	2.32	0.62
1:C:119:LYS:HG2	1:C:120:VAL:N	2.14	0.62
1:B:127:VAL:CG1	1:B:129:ASP:H	2.13	0.62
1:C:483:ALA:HB3	1:C:484:LYS:HE3	1.80	0.62
1:A:186:PRO:HB2	3:A:512:HOH:O	2.00	0.62
1:A:187:VAL:CG1	1:A:341:ILE:HD12	2.29	0.62
1:E:287:GLN:H	1:E:287:GLN:HE21	1.48	0.62
1:D:483:ALA:HB3	1:D:484:LYS:HE3	1.82	0.62
1:D:187:VAL:CG1	1:D:341:ILE:HD12	2.30	0.62
1:E:167:ILE:HD11	1:E:318:TYR:CE2	2.35	0.62
1:B:187:VAL:CG1	1:B:341:ILE:HD12	2.30	0.62
1:F:24:SER:HB3	1:F:125:ILE:HG22	1.80	0.62
1:F:26:PHE:HB3	1:F:306:SER:HB3	1.82	0.62
1:C:167:ILE:HD11	1:C:318:TYR:CE2	2.34	0.62
1:C:189:THR:HG22	1:C:191:SER:H	1.65	0.62
1:A:119:LYS:HG2	1:A:120:VAL:N	2.14	0.62
1:E:435:ASN:HD21	1:E:438:GLU:H	1.48	0.61
1:B:294:MSE:HE2	1:B:324:PHE:CD2	2.34	0.61
1:A:435:ASN:HD21	1:A:438:GLU:H	1.47	0.61
1:A:287:GLN:H	1:A:287:GLN:HE21	1.48	0.61
1:F:411:HIS:HA	3:F:523:HOH:O	1.99	0.61
1:E:311:ARG:O	1:E:315:GLN:HG3	2.00	0.61
1:B:119:LYS:HG2	1:B:120:VAL:N	2.14	0.61
1:A:256:GLN:HA	1:A:283:THR:HG23	1.82	0.61
1:E:119:LYS:HG2	1:E:120:VAL:N	2.13	0.61
1:D:287:GLN:HE21	1:D:287:GLN:H	1.49	0.61
1:A:189:THR:HG22	1:A:191:SER:H	1.66	0.61
1:D:26:PHE:HB3	1:D:306:SER:HB3	1.83	0.61
1:F:483:ALA:HB3	1:F:484:LYS:HE3	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:167:ILE:HD11	1:D:318:TYR:CE2	2.35	0.61
1:B:412:HIS:CD2	3:B:512:HOH:O	2.52	0.61
1:C:294:MSE:HE2	1:C:324:PHE:CD2	2.35	0.61
1:B:167:ILE:HD11	1:B:318:TYR:CE2	2.36	0.61
1:B:435:ASN:HD21	1:B:438:GLU:H	1.48	0.61
1:C:435:ASN:C	1:C:435:ASN:HD22	2.03	0.61
1:C:94:ASN:HD21	1:C:372:MSE:N	1.94	0.60
1:D:256:GLN:HA	1:D:283:THR:HG23	1.82	0.60
1:C:287:GLN:H	1:C:287:GLN:HE21	1.49	0.60
1:D:189:THR:HG22	1:D:191:SER:H	1.66	0.60
1:F:93:ILE:HG12	3:F:543:HOH:O	2.01	0.60
1:B:410:ALA:N	3:B:524:HOH:O	2.33	0.60
1:C:163:HIS:HD2	1:C:318:TYR:OH	1.83	0.60
1:F:187:VAL:HG13	1:F:341:ILE:HD12	1.82	0.60
1:A:167:ILE:HD11	1:A:318:TYR:CE2	2.36	0.60
1:D:127:VAL:CG1	1:D:129:ASP:H	2.13	0.60
1:C:259:VAL:HG22	3:C:516:HOH:O	2.01	0.60
1:B:256:GLN:HA	1:B:283:THR:HG23	1.81	0.60
1:F:27:THR:HG22	3:F:535:HOH:O	2.01	0.60
1:F:94:ASN:HD21	1:F:372:MSE:N	1.96	0.59
1:F:454:PRO:HG2	3:F:513:HOH:O	2.02	0.59
1:D:82:PRO:O	1:D:102:ASP:HA	2.02	0.59
1:E:82:PRO:O	1:E:102:ASP:HA	2.03	0.59
1:D:94:ASN:HD21	1:D:372:MSE:N	1.96	0.59
1:F:187:VAL:CG1	1:F:341:ILE:HD12	2.33	0.59
1:F:257:SER:H	1:F:283:THR:HG22	1.67	0.59
1:E:94:ASN:HD21	1:E:372:MSE:N	1.97	0.59
1:F:82:PRO:O	1:F:102:ASP:HA	2.03	0.59
1:E:483:ALA:HB3	1:E:484:LYS:HE3	1.84	0.59
1:E:427:GLY:N	3:E:515:HOH:O	2.36	0.59
1:F:256:GLN:HA	1:F:283:THR:HG23	1.83	0.59
1:A:249:PRO:HG2	1:A:253:LEU:HD13	1.84	0.59
1:D:119:LYS:HG2	1:D:120:VAL:N	2.16	0.59
1:C:467:GLN:H	1:D:94:ASN:HD22	1.50	0.59
1:E:249:PRO:HG2	1:E:253:LEU:HD13	1.85	0.59
1:C:256:GLN:HA	1:C:283:THR:HG23	1.82	0.59
1:E:117:TYR:O	1:E:118:GLY:O	2.21	0.58
1:F:311:ARG:O	1:F:315:GLN:HG3	2.03	0.58
1:B:34:VAL:N	3:B:513:HOH:O	2.33	0.58
1:C:448:VAL:O	1:C:453:ARG:HD3	2.02	0.58
1:B:82:PRO:O	1:B:102:ASP:HA	2.02	0.58
1:B:362:ILE:HD13	1:B:419:VAL:HG21	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:359:PHE:O	1:E:439:ARG:HD2	2.03	0.58
1:F:249:PRO:HG2	1:F:253:LEU:HD13	1.85	0.58
1:A:90:ARG:HD3	1:A:373:MSE:O	2.03	0.58
1:E:127:VAL:HG13	1:E:137:LEU:O	2.04	0.58
1:F:435:ASN:HD21	1:F:438:GLU:H	1.50	0.58
1:B:287:GLN:NE2	1:B:287:GLN:H	2.02	0.58
1:A:311:ARG:O	1:A:315:GLN:HG3	2.04	0.58
1:F:421:VAL:HG13	3:F:514:HOH:O	2.04	0.58
1:B:435:ASN:HD22	1:B:435:ASN:C	2.07	0.58
1:A:82:PRO:O	1:A:102:ASP:HA	2.04	0.57
1:C:287:GLN:HB3	3:C:516:HOH:O	2.05	0.57
1:B:249:PRO:HG2	1:B:253:LEU:HD13	1.85	0.57
1:B:359:PHE:O	1:B:439:ARG:HD2	2.05	0.57
1:C:359:PHE:O	1:C:439:ARG:HD2	2.05	0.57
1:C:362:ILE:HD13	1:C:419:VAL:HG21	1.86	0.57
1:A:257:SER:H	1:A:283:THR:HG22	1.69	0.57
1:B:311:ARG:O	1:B:315:GLN:HG3	2.03	0.57
1:B:189:THR:HG22	1:B:191:SER:H	1.69	0.57
1:F:189:THR:HG22	1:F:191:SER:H	1.70	0.57
1:E:349:THR:HG23	1:E:386:SER:HB3	1.87	0.57
1:A:487:ASP:OD1	1:A:489:ARG:HD3	2.04	0.56
1:E:185:LEU:HB2	1:E:341:ILE:HD11	1.88	0.56
1:C:311:ARG:O	1:C:315:GLN:HG3	2.04	0.56
1:C:249:PRO:HG2	1:C:253:LEU:HD13	1.86	0.56
1:E:435:ASN:C	1:E:435:ASN:HD22	2.09	0.56
1:A:435:ASN:HD22	1:A:435:ASN:C	2.07	0.56
1:B:225:ASP:OD2	1:B:228:THR:HG23	2.05	0.56
1:F:90:ARG:HD3	1:F:373:MSE:O	2.04	0.56
1:E:358:ILE:O	1:E:440:ALA:HA	2.06	0.56
1:B:90:ARG:HD3	1:B:373:MSE:O	2.05	0.56
1:B:94:ASN:HD21	1:B:372:MSE:N	1.98	0.56
1:B:117:TYR:O	1:B:118:GLY:O	2.24	0.56
1:E:90:ARG:HD3	1:E:373:MSE:O	2.05	0.56
1:E:257:SER:H	1:E:283:THR:HG22	1.70	0.56
1:C:82:PRO:O	1:C:102:ASP:HA	2.06	0.56
1:F:435:ASN:HD22	1:F:435:ASN:C	2.08	0.56
1:F:233:ASP:HB3	3:F:530:HOH:O	2.05	0.56
1:F:225:ASP:OD2	1:F:228:THR:HG23	2.06	0.56
1:C:487:ASP:OD1	1:C:489:ARG:HD3	2.05	0.56
1:F:185:LEU:HB2	1:F:341:ILE:HD11	1.87	0.56
1:C:218:GLU:HG3	1:C:219:SER:N	2.21	0.56
1:F:448:VAL:O	1:F:453:ARG:HD3	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:448:VAL:O	1:E:453:ARG:HD3	2.06	0.55
1:C:257:SER:H	1:C:283:THR:HG22	1.72	0.55
1:E:294:MSE:HE3	1:E:327:LYS:CB	2.35	0.55
1:D:257:SER:H	1:D:283:THR:HG22	1.70	0.55
1:A:185:LEU:HB2	1:A:341:ILE:HD11	1.88	0.55
1:E:487:ASP:OD1	1:E:489:ARG:HD3	2.05	0.55
1:E:77:VAL:HG22	3:E:555:HOH:O	2.05	0.55
1:F:127:VAL:HG13	1:F:137:LEU:O	2.05	0.55
1:F:338:ASN:O	1:F:342:VAL:HG23	2.06	0.55
1:E:225:ASP:OD2	1:E:228:THR:HG23	2.06	0.55
1:D:185:LEU:HB2	1:D:341:ILE:HD11	1.89	0.55
1:F:349:THR:HG23	1:F:386:SER:HB3	1.88	0.55
1:E:36:PRO:HG3	1:E:67:LEU:HD22	1.88	0.55
1:E:393:THR:HG22	3:E:553:HOH:O	2.06	0.55
1:A:349:THR:HG23	1:A:386:SER:HB3	1.88	0.55
1:E:221:PHE:CE1	1:E:223:PRO:HB3	2.42	0.55
1:A:448:VAL:O	1:A:453:ARG:HD3	2.07	0.55
1:C:185:LEU:HB2	1:C:341:ILE:HD11	1.88	0.55
1:C:225:ASP:OD2	1:C:228:THR:HG23	2.07	0.55
1:A:359:PHE:O	1:A:439:ARG:HD2	2.06	0.55
1:A:218:GLU:HG3	1:A:219:SER:N	2.22	0.55
1:A:225:ASP:OD2	1:A:228:THR:HG23	2.06	0.54
1:A:362:ILE:HD13	1:A:419:VAL:HG21	1.90	0.54
1:D:90:ARG:HD3	1:D:373:MSE:O	2.06	0.54
1:B:36:PRO:HG3	1:B:67:LEU:HD22	1.89	0.54
1:D:127:VAL:HG13	1:D:137:LEU:O	2.07	0.54
1:D:358:ILE:O	1:D:440:ALA:HA	2.08	0.54
1:D:435:ASN:HD22	1:D:435:ASN:C	2.09	0.54
1:A:117:TYR:O	1:A:118:GLY:O	2.25	0.54
1:B:131:THR:CG2	1:B:133:ASP:OD1	2.55	0.54
1:E:216:ASN:ND2	3:E:538:HOH:O	2.40	0.54
1:C:387:TYR:HE2	1:D:179:PRO:HG2	1.73	0.54
1:C:435:ASN:C	1:C:435:ASN:ND2	2.61	0.54
1:D:249:PRO:HG2	1:D:253:LEU:HD13	1.88	0.54
1:B:349:THR:HG23	1:B:386:SER:HB3	1.90	0.54
1:F:81:THR:HG22	1:F:82:PRO:CA	2.36	0.54
1:D:487:ASP:OD1	1:D:489:ARG:HD3	2.07	0.54
1:F:359:PHE:O	1:F:439:ARG:HD2	2.08	0.54
1:A:356:ALA:HB1	3:A:536:HOH:O	2.06	0.54
1:F:30:GLY:HA2	1:F:139:THR:OG1	2.06	0.54
1:A:358:ILE:O	1:A:440:ALA:HA	2.08	0.54
1:F:287:GLN:NE2	1:F:290:VAL:HG23	2.23	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:362:ILE:HD13	1:D:419:VAL:HG21	1.90	0.54
1:C:90:ARG:HD3	1:C:373:MSE:O	2.07	0.54
1:B:358:ILE:O	1:B:440:ALA:HA	2.07	0.54
1:C:92:LEU:HD12	1:C:97:SER:HB2	1.90	0.54
1:A:127:VAL:HG13	1:A:137:LEU:O	2.08	0.54
1:C:349:THR:HG23	1:C:386:SER:HB3	1.90	0.54
1:F:435:ASN:ND2	1:F:438:GLU:HG3	2.21	0.54
1:B:487:ASP:OD1	1:B:489:ARG:HD3	2.07	0.54
1:F:309:VAL:HA	3:F:525:HOH:O	2.08	0.54
1:D:359:PHE:O	1:D:439:ARG:HD2	2.07	0.54
1:A:92:LEU:HD12	1:A:97:SER:HB2	1.90	0.54
1:B:257:SER:H	1:B:283:THR:HG22	1.72	0.54
1:D:81:THR:HG22	1:D:82:PRO:CA	2.36	0.54
1:F:117:TYR:O	1:F:118:GLY:O	2.26	0.54
1:D:130:VAL:O	1:D:130:VAL:HG13	2.08	0.54
1:B:127:VAL:HG13	1:B:137:LEU:O	2.08	0.53
1:C:358:ILE:O	1:C:440:ALA:HA	2.08	0.53
1:D:448:VAL:O	1:D:453:ARG:HD3	2.09	0.53
1:B:185:LEU:HB2	1:B:341:ILE:HD11	1.89	0.53
1:A:36:PRO:HG3	1:A:67:LEU:HD22	1.90	0.53
1:B:294:MSE:CE	1:B:327:LYS:HB2	2.39	0.53
1:E:287:GLN:H	1:E:287:GLN:NE2	2.06	0.53
1:D:287:GLN:NE2	1:D:287:GLN:H	2.07	0.53
1:D:117:TYR:O	1:D:118:GLY:O	2.27	0.53
1:D:225:ASP:OD2	1:D:228:THR:HG23	2.08	0.53
1:C:117:TYR:O	1:C:118:GLY:O	2.27	0.53
1:A:30:GLY:HA2	1:A:139:THR:OG1	2.09	0.53
1:F:161:ASP:HB2	1:F:213:SER:HA	1.91	0.53
1:E:435:ASN:ND2	1:E:438:GLU:HG3	2.21	0.53
1:B:161:ASP:HB2	1:B:213:SER:HA	1.91	0.53
1:F:362:ILE:HD13	1:F:419:VAL:HG21	1.91	0.53
1:D:281:MSE:HE3	1:D:283:THR:CG2	2.39	0.53
1:D:349:THR:HG23	1:D:386:SER:HB3	1.90	0.53
1:C:287:GLN:H	1:C:287:GLN:NE2	2.07	0.53
1:D:131:THR:CG2	1:D:133:ASP:OD1	2.57	0.53
1:E:30:GLY:HA2	1:E:139:THR:OG1	2.07	0.53
1:D:161:ASP:HB2	1:D:213:SER:HA	1.90	0.53
1:F:440:ALA:O	1:F:444:ILE:HG13	2.08	0.53
1:B:130:VAL:O	1:B:130:VAL:HG13	2.09	0.53
1:B:448:VAL:O	1:B:453:ARG:HD3	2.08	0.52
1:C:179:PRO:HG2	1:D:387:TYR:HE2	1.75	0.52
1:C:81:THR:HG22	1:C:82:PRO:CA	2.37	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:355:GLU:OE1	1:E:479:HIS:HE1	1.92	0.52
1:F:287:GLN:HE21	1:F:287:GLN:H	1.55	0.52
1:B:30:GLY:HA2	1:B:139:THR:OG1	2.08	0.52
1:A:280:ASN:ND2	1:A:301:PHE:HB3	2.24	0.52
1:E:415:SER:HB2	3:F:541:HOH:O	2.09	0.52
1:D:30:GLY:HA2	1:D:139:THR:OG1	2.09	0.52
1:A:287:GLN:H	1:A:287:GLN:NE2	2.07	0.52
1:E:362:ILE:HD13	1:E:419:VAL:HG21	1.91	0.52
1:E:221:PHE:CE1	1:E:223:PRO:HD3	2.44	0.52
1:C:255:LEU:HD23	1:C:348:ILE:HB	1.90	0.52
1:E:131:THR:HG22	1:E:132:GLU:N	2.25	0.52
1:F:331:ARG:NH1	3:F:527:HOH:O	2.43	0.52
1:C:30:GLY:HA2	1:C:139:THR:OG1	2.09	0.52
1:A:81:THR:HG22	1:A:82:PRO:CA	2.37	0.52
1:E:340:GLU:CG	1:F:340:GLU:HG3	2.37	0.52
1:D:218:GLU:HG3	1:D:219:SER:N	2.25	0.52
1:B:17:HIS:HD2	1:B:54:LYS:N	2.03	0.52
1:E:77:VAL:HA	3:E:555:HOH:O	2.09	0.52
1:D:320:ASN:HA	1:D:322:ASP:OD1	2.09	0.52
1:F:287:GLN:NE2	1:F:287:GLN:H	2.08	0.52
1:C:161:ASP:HB2	1:C:213:SER:HA	1.92	0.52
1:E:294:MSE:CE	1:E:327:LYS:HB2	2.38	0.52
1:A:161:ASP:HB2	1:A:213:SER:HA	1.92	0.52
1:F:237:ALA:HA	3:F:511:HOH:O	2.10	0.52
1:E:161:ASP:HB2	1:E:213:SER:HA	1.92	0.51
1:F:320:ASN:HA	1:F:322:ASP:OD1	2.10	0.51
1:D:92:LEU:HD12	1:D:97:SER:HB2	1.92	0.51
1:E:138:PRO:HG3	1:E:145:LEU:CD2	2.41	0.51
1:F:69:GLY:O	1:F:73:GLN:HG3	2.10	0.51
1:F:92:LEU:HD12	1:F:97:SER:HB2	1.92	0.51
1:C:36:PRO:HG3	1:C:67:LEU:HD22	1.92	0.51
1:E:281:MSE:HE3	1:E:283:THR:CG2	2.41	0.51
1:F:187:VAL:HB	3:F:512:HOH:O	2.10	0.51
1:B:81:THR:HG22	1:B:82:PRO:CA	2.39	0.51
1:F:487:ASP:OD1	1:F:489:ARG:HD3	2.10	0.51
1:A:81:THR:CG2	1:A:82:PRO:HA	2.40	0.51
1:F:131:THR:CG2	1:F:133:ASP:OD1	2.58	0.51
1:D:36:PRO:HG3	1:D:67:LEU:HD22	1.91	0.51
1:C:127:VAL:HG13	1:C:137:LEU:O	2.11	0.51
1:D:338:ASN:O	1:D:342:VAL:HG23	2.11	0.51
1:D:81:THR:CG2	1:D:82:PRO:HA	2.38	0.51
1:D:271:GLY:HA2	1:D:298:ARG:HD2	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:281:MSE:HE3	1:F:283:THR:CG2	2.40	0.51
1:F:453:ARG:HD2	3:F:515:HOH:O	2.09	0.51
1:C:338:ASN:O	1:C:342:VAL:HG23	2.11	0.51
1:E:349:THR:CG2	1:E:386:SER:HB3	2.41	0.51
1:E:218:GLU:HG3	1:E:219:SER:N	2.26	0.51
1:B:280:ASN:ND2	1:B:301:PHE:HB3	2.26	0.51
1:D:294:MSE:CE	1:D:327:LYS:HB2	2.36	0.50
1:C:280:ASN:ND2	1:C:301:PHE:HB3	2.26	0.50
1:B:435:ASN:ND2	1:B:438:GLU:HG3	2.24	0.50
1:C:67:LEU:O	1:C:71:LEU:HB2	2.12	0.50
1:B:255:LEU:HD23	1:B:348:ILE:HB	1.93	0.50
1:E:255:LEU:HD23	1:E:348:ILE:HB	1.92	0.50
1:A:256:GLN:HG3	1:A:382:PHE:CE1	2.47	0.50
1:F:358:ILE:O	1:F:440:ALA:HA	2.10	0.50
1:E:340:GLU:HG3	1:F:340:GLU:CG	2.38	0.50
1:D:440:ALA:O	1:D:444:ILE:HG13	2.11	0.50
1:E:338:ASN:O	1:E:342:VAL:HG23	2.12	0.50
1:A:255:LEU:HD23	1:A:348:ILE:HB	1.92	0.50
1:C:131:THR:HG22	1:C:132:GLU:N	2.26	0.50
1:C:440:ALA:O	1:C:444:ILE:HG13	2.10	0.50
1:E:320:ASN:HA	1:E:322:ASP:OD1	2.12	0.50
1:A:281:MSE:HE3	1:A:283:THR:CG2	2.41	0.50
1:E:435:ASN:ND2	1:E:435:ASN:C	2.65	0.50
1:B:320:ASN:HA	1:B:322:ASP:OD1	2.11	0.50
1:F:17:HIS:HD2	1:F:54:LYS:N	2.02	0.50
1:F:81:THR:CG2	1:F:82:PRO:HA	2.38	0.50
1:B:81:THR:CG2	1:B:82:PRO:HA	2.41	0.50
1:B:92:LEU:HD12	1:B:97:SER:HB2	1.94	0.50
1:D:280:ASN:ND2	1:D:301:PHE:HB3	2.26	0.50
1:A:131:THR:HG22	1:A:132:GLU:N	2.27	0.50
1:A:440:ALA:O	1:A:444:ILE:HG13	2.12	0.50
1:F:281:MSE:HE3	1:F:283:THR:HG23	1.94	0.50
1:F:349:THR:CG2	1:F:386:SER:HB3	2.42	0.50
1:E:130:VAL:HG13	1:E:130:VAL:O	2.12	0.50
1:F:421:VAL:N	3:F:517:HOH:O	2.45	0.50
1:A:435:ASN:ND2	1:A:435:ASN:C	2.65	0.50
1:F:355:GLU:OE1	1:F:479:HIS:HE1	1.95	0.50
1:C:281:MSE:HE3	1:C:283:THR:CG2	2.42	0.49
1:A:131:THR:CG2	1:A:133:ASP:OD1	2.60	0.49
1:A:37:ALA:HB2	3:A:519:HOH:O	2.12	0.49
1:D:255:LEU:HD23	1:D:348:ILE:HB	1.92	0.49
1:E:448:VAL:HG23	3:E:541:HOH:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:355:GLU:OE1	1:B:479:HIS:HE1	1.95	0.49
1:E:131:THR:CG2	1:E:133:ASP:OD1	2.60	0.49
1:F:255:LEU:HD23	1:F:348:ILE:HB	1.94	0.49
1:D:281:MSE:HE3	1:D:283:THR:HG23	1.95	0.49
1:F:36:PRO:HG3	1:F:67:LEU:HD22	1.94	0.49
1:C:130:VAL:HG13	1:C:130:VAL:O	2.13	0.49
1:E:349:THR:CG2	1:E:382:PHE:HB3	2.42	0.49
1:A:435:ASN:ND2	1:A:438:GLU:HG3	2.27	0.49
1:D:35:VAL:N	1:D:36:PRO:HD2	2.27	0.49
1:F:67:LEU:O	1:F:71:LEU:HB2	2.13	0.49
1:C:138:PRO:HG3	1:C:145:LEU:CD2	2.43	0.49
1:F:429:ALA:O	1:F:431:LEU:HD13	2.12	0.49
1:C:17:HIS:HD2	1:C:54:LYS:N	2.05	0.49
1:D:435:ASN:ND2	1:D:438:GLU:HG3	2.25	0.49
1:A:454:PRO:HG2	3:A:531:HOH:O	2.12	0.49
1:B:349:THR:CG2	1:B:386:SER:HB3	2.43	0.49
1:F:331:ARG:HB3	3:F:537:HOH:O	2.12	0.49
1:C:81:THR:CG2	1:C:82:PRO:HA	2.39	0.49
1:A:338:ASN:O	1:A:342:VAL:HG23	2.13	0.49
1:E:92:LEU:HD12	1:E:97:SER:HB2	1.95	0.49
1:E:429:ALA:O	1:E:431:LEU:HD13	2.13	0.49
1:F:130:VAL:O	1:F:130:VAL:HG13	2.13	0.49
1:C:354:LEU:HD11	1:C:373:MSE:HG3	1.95	0.49
1:D:435:ASN:ND2	1:D:435:ASN:C	2.66	0.49
1:C:435:ASN:ND2	1:C:438:GLU:HG3	2.26	0.49
1:A:138:PRO:HG3	1:A:145:LEU:CD2	2.43	0.49
1:E:435:ASN:ND2	1:E:438:GLU:CG	2.76	0.49
1:E:280:ASN:ND2	1:E:301:PHE:HB3	2.28	0.49
1:A:280:ASN:HD22	1:A:301:PHE:HB3	1.78	0.49
1:F:271:GLY:HA2	1:F:298:ARG:HD2	1.94	0.48
1:B:435:ASN:ND2	1:B:435:ASN:C	2.66	0.48
1:E:69:GLY:O	1:E:73:GLN:HG3	2.13	0.48
1:A:397:MSE:HG2	1:A:398:LYS:N	2.28	0.48
1:B:35:VAL:N	1:B:36:PRO:HD2	2.29	0.48
1:D:349:THR:CG2	1:D:382:PHE:HB3	2.43	0.48
1:C:340:GLU:HG3	1:D:340:GLU:CG	2.41	0.48
1:E:221:PHE:CD1	1:E:223:PRO:HD3	2.47	0.48
1:B:131:THR:HG22	1:B:132:GLU:N	2.29	0.48
1:C:94:ASN:ND2	1:C:372:MSE:H	1.99	0.48
1:D:349:THR:CG2	1:D:386:SER:HB3	2.44	0.48
1:A:294:MSE:CE	1:A:327:LYS:HB2	2.40	0.48
1:D:318:TYR:HA	1:D:321:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:361:ASN:C	1:B:362:ILE:HD12	2.33	0.48
1:E:236:ALA:O	1:E:240:VAL:HG13	2.14	0.48
1:A:281:MSE:HE3	1:A:283:THR:HG23	1.95	0.48
1:C:349:THR:CG2	1:C:382:PHE:HB3	2.41	0.48
1:F:435:ASN:ND2	1:F:435:ASN:C	2.66	0.48
1:C:293:LEU:O	1:C:298:ARG:HB3	2.14	0.48
1:C:318:TYR:HA	1:C:321:LEU:CD1	2.43	0.48
1:C:69:GLY:O	1:C:73:GLN:HG3	2.13	0.48
1:A:271:GLY:HA2	1:A:298:ARG:HD2	1.94	0.48
1:F:280:ASN:ND2	1:F:301:PHE:HB3	2.29	0.48
1:D:138:PRO:HG3	1:D:145:LEU:CD2	2.44	0.48
1:A:293:LEU:O	1:A:298:ARG:HB3	2.14	0.48
1:E:440:ALA:O	1:E:444:ILE:HG13	2.14	0.48
1:E:81:THR:HG22	1:E:82:PRO:CA	2.39	0.48
1:E:81:THR:CG2	1:E:82:PRO:HA	2.41	0.48
1:E:271:GLY:HA2	1:E:298:ARG:HD2	1.96	0.48
1:C:429:ALA:O	1:C:431:LEU:HD13	2.13	0.48
1:D:17:HIS:HD2	1:D:54:LYS:N	2.03	0.48
1:B:318:TYR:HA	1:B:321:LEU:CD1	2.43	0.48
1:D:280:ASN:HD22	1:D:301:PHE:HB3	1.78	0.48
1:B:423:ILE:HG12	1:B:428:VAL:HB	1.96	0.48
1:D:69:GLY:O	1:D:73:GLN:HG3	2.14	0.48
1:B:33:LYS:N	3:B:513:HOH:O	2.45	0.48
1:A:349:THR:CG2	1:A:386:SER:HB3	2.43	0.48
1:F:349:THR:CG2	1:F:382:PHE:HB3	2.42	0.48
1:C:355:GLU:OE1	1:C:479:HIS:HE1	1.96	0.48
1:A:429:ALA:O	1:A:431:LEU:HD13	2.13	0.48
1:B:218:GLU:HG3	1:B:219:SER:N	2.28	0.48
1:C:349:THR:CG2	1:C:386:SER:HB3	2.44	0.48
1:D:131:THR:HG22	1:D:132:GLU:N	2.29	0.48
1:C:89:LEU:O	1:C:93:ILE:HG13	2.13	0.48
1:A:69:GLY:O	1:A:73:GLN:HG3	2.14	0.48
1:A:67:LEU:O	1:A:71:LEU:HB2	2.13	0.47
1:F:131:THR:HG22	1:F:132:GLU:N	2.29	0.47
1:C:94:ASN:HD22	1:D:467:GLN:H	1.61	0.47
1:B:67:LEU:O	1:B:71:LEU:HB2	2.14	0.47
1:C:320:ASN:HA	1:C:322:ASP:OD1	2.13	0.47
1:C:131:THR:CG2	1:C:133:ASP:OD1	2.63	0.47
1:A:320:ASN:HA	1:A:322:ASP:OD1	2.14	0.47
1:C:340:GLU:CG	1:D:340:GLU:HG3	2.42	0.47
1:E:35:VAL:N	1:E:36:PRO:HD2	2.30	0.47
1:F:27:THR:HA	1:F:62:SER:OG	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:221:PHE:CZ	1:E:223:PRO:HG3	2.50	0.47
1:B:280:ASN:HD22	1:B:301:PHE:HB3	1.79	0.47
1:B:27:THR:HA	1:B:62:SER:OG	2.14	0.47
1:B:281:MSE:HE3	1:B:283:THR:CG2	2.44	0.47
1:C:281:MSE:HE3	1:C:283:THR:HG23	1.96	0.47
1:D:256:GLN:HG3	1:D:382:PHE:CE1	2.49	0.47
1:C:294:MSE:CE	1:C:327:LYS:HB2	2.39	0.47
1:F:294:MSE:CE	1:F:327:LYS:HB2	2.39	0.47
1:E:301:PHE:N	3:E:556:HOH:O	2.47	0.47
1:A:318:TYR:HA	1:A:321:LEU:CD1	2.44	0.47
1:A:355:GLU:OE1	1:A:479:HIS:HE1	1.96	0.47
1:F:89:LEU:O	1:F:93:ILE:HG13	2.14	0.47
1:F:287:GLN:HE21	1:F:290:VAL:HG23	1.80	0.47
1:B:89:LEU:O	1:B:93:ILE:HG13	2.14	0.47
1:C:92:LEU:CD1	1:C:97:SER:HB2	2.45	0.47
1:F:37:ALA:O	1:F:41:LYS:HG2	2.15	0.47
1:C:481:GLU:OE1	1:C:485:SER:OG	2.30	0.47
1:B:256:GLN:HG3	1:B:382:PHE:CE1	2.49	0.47
1:C:271:GLY:HA2	1:C:298:ARG:HD2	1.96	0.47
1:E:17:HIS:HD2	1:E:54:LYS:N	2.02	0.47
1:B:349:THR:CG2	1:B:382:PHE:HB3	2.43	0.47
1:A:349:THR:CG2	1:A:382:PHE:HB3	2.44	0.47
1:E:276:ILE:O	1:E:298:ARG:NH1	2.48	0.47
1:F:257:SER:H	1:F:283:THR:CG2	2.26	0.47
1:F:318:TYR:HA	1:F:321:LEU:CD1	2.44	0.47
1:F:435:ASN:HD21	1:F:438:GLU:CG	2.26	0.47
1:E:9:GLU:HB2	3:E:557:HOH:O	2.14	0.47
1:A:130:VAL:HG13	1:A:130:VAL:O	2.14	0.47
1:A:298:ARG:NE	3:A:516:HOH:O	2.16	0.47
1:E:318:TYR:HA	1:E:321:LEU:CD1	2.44	0.47
1:C:186:PRO:HG2	1:C:194:ILE:CG2	2.45	0.47
1:A:17:HIS:HD2	1:A:54:LYS:N	2.03	0.46
1:F:256:GLN:HG3	1:F:382:PHE:CE1	2.50	0.46
1:F:435:ASN:ND2	1:F:438:GLU:CG	2.78	0.46
1:A:423:ILE:HG12	1:A:428:VAL:HB	1.98	0.46
1:D:397:MSE:HG2	1:D:398:LYS:N	2.30	0.46
1:E:27:THR:HA	1:E:62:SER:OG	2.14	0.46
1:F:79:PHE:C	1:F:79:PHE:CD1	2.89	0.46
1:D:186:PRO:HG2	1:D:194:ILE:CG2	2.45	0.46
1:A:298:ARG:CB	3:A:516:HOH:O	2.35	0.46
1:B:440:ALA:O	1:B:444:ILE:HG13	2.14	0.46
1:F:271:GLY:HA2	1:F:298:ARG:CD	2.44	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:PHE:CE1	1:A:61:ALA:HB2	2.51	0.46
1:C:361:ASN:C	1:C:362:ILE:HD12	2.35	0.46
1:D:361:ASN:C	1:D:362:ILE:HD12	2.36	0.46
1:C:280:ASN:HD22	1:C:301:PHE:HB3	1.80	0.46
1:F:397:MSE:HG2	1:F:398:LYS:N	2.30	0.46
1:B:69:GLY:O	1:B:73:GLN:HG3	2.15	0.46
1:F:35:VAL:N	1:F:36:PRO:HD2	2.30	0.46
1:C:423:ILE:HG12	1:C:428:VAL:HB	1.98	0.46
1:D:79:PHE:CD1	1:D:79:PHE:C	2.89	0.46
1:E:79:PHE:C	1:E:79:PHE:CD1	2.89	0.46
1:A:271:GLY:HA2	1:A:298:ARG:CD	2.45	0.46
1:E:448:VAL:N	3:E:541:HOH:O	2.47	0.46
1:E:281:MSE:HE3	1:E:283:THR:HG23	1.98	0.46
1:D:276:ILE:O	1:D:298:ARG:NH1	2.48	0.46
1:B:271:GLY:HA2	1:B:298:ARG:HD2	1.96	0.46
1:F:355:GLU:HG3	1:F:409:VAL:HG12	1.98	0.46
1:D:355:GLU:OE1	1:D:479:HIS:HE1	1.99	0.46
1:D:36:PRO:HG2	3:D:512:HOH:O	2.16	0.46
1:D:27:THR:HA	1:D:62:SER:OG	2.14	0.46
1:B:236:ALA:O	1:B:240:VAL:HG13	2.15	0.46
1:C:256:GLN:HG3	1:C:382:PHE:CE1	2.50	0.46
1:E:355:GLU:HG3	1:E:409:VAL:HG12	1.98	0.46
1:B:138:PRO:HG3	1:B:145:LEU:CD2	2.45	0.46
1:F:218:GLU:HG3	1:F:219:SER:N	2.30	0.46
1:A:257:SER:H	1:A:283:THR:CG2	2.28	0.46
1:C:287:GLN:NE2	1:C:290:VAL:HG23	2.31	0.46
1:F:138:PRO:HG3	1:F:145:LEU:CD2	2.45	0.46
1:D:54:LYS:HG2	1:D:76:ALA:HA	1.98	0.46
1:D:257:SER:H	1:D:283:THR:CG2	2.28	0.46
1:E:435:ASN:HD21	1:E:438:GLU:CG	2.23	0.46
1:D:271:GLY:HA2	1:D:298:ARG:CD	2.46	0.46
1:A:4:ARG:NH1	3:A:529:HOH:O	2.44	0.46
1:F:221:PHE:CE1	1:F:223:PRO:HB3	2.51	0.46
1:E:186:PRO:HG2	1:E:194:ILE:CG2	2.46	0.46
1:A:354:LEU:HD11	1:A:373:MSE:HG3	1.98	0.46
1:D:321:LEU:O	1:D:325:LYS:HB2	2.16	0.46
1:F:403:SER:H	1:F:488:MSE:SE	2.49	0.46
1:E:467:GLN:H	1:F:94:ASN:HD22	1.63	0.46
1:B:338:ASN:O	1:B:342:VAL:HG23	2.16	0.46
1:D:63:THR:HB	1:D:67:LEU:HG	1.98	0.46
1:F:423:ILE:HG12	1:F:428:VAL:HB	1.98	0.46
1:B:321:LEU:O	1:B:325:LYS:HB2	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:441:HIS:HE1	3:B:516:HOH:O	1.98	0.45
1:B:37:ALA:O	1:B:41:LYS:HG2	2.16	0.45
1:C:397:MSE:HG2	1:C:398:LYS:N	2.31	0.45
1:E:94:ASN:HD22	1:F:467:GLN:H	1.62	0.45
1:C:257:SER:H	1:C:283:THR:CG2	2.29	0.45
1:E:271:GLY:HA2	1:E:298:ARG:CD	2.45	0.45
1:B:276:ILE:O	1:B:298:ARG:NH1	2.49	0.45
1:E:67:LEU:O	1:E:71:LEU:HB2	2.16	0.45
1:F:26:PHE:CE1	1:F:61:ALA:HB2	2.50	0.45
1:A:92:LEU:CD1	1:A:97:SER:HB2	2.46	0.45
1:F:221:PHE:CE1	1:F:223:PRO:HD3	2.51	0.45
1:E:403:SER:H	1:E:488:MSE:SE	2.49	0.45
1:D:429:ALA:O	1:D:431:LEU:HD13	2.15	0.45
1:F:354:LEU:HD11	1:F:373:MSE:HG3	1.98	0.45
1:B:435:ASN:ND2	1:B:438:GLU:CG	2.79	0.45
1:E:280:ASN:HD22	1:E:301:PHE:HB3	1.81	0.45
1:F:186:PRO:HG2	1:F:194:ILE:CG2	2.46	0.45
1:B:429:ALA:O	1:B:431:LEU:HD13	2.15	0.45
1:D:89:LEU:O	1:D:93:ILE:HG13	2.16	0.45
1:B:453:ARG:O	1:B:457:ARG:HG3	2.17	0.45
1:F:321:LEU:O	1:F:325:LYS:HB2	2.16	0.45
1:E:26:PHE:CE1	1:E:61:ALA:HB2	2.51	0.45
1:A:35:VAL:N	1:A:36:PRO:HD2	2.31	0.45
1:D:423:ILE:HG12	1:D:428:VAL:HB	1.99	0.45
1:A:94:ASN:ND2	1:A:372:MSE:H	2.00	0.45
1:E:354:LEU:HD11	1:E:373:MSE:HG3	1.98	0.45
1:F:293:LEU:O	1:F:298:ARG:HB3	2.17	0.45
1:E:321:LEU:O	1:E:325:LYS:HB2	2.16	0.45
1:E:423:ILE:HG12	1:E:428:VAL:HB	1.99	0.45
1:C:271:GLY:HA2	1:C:298:ARG:CD	2.47	0.45
1:C:26:PHE:CE1	1:C:61:ALA:HB2	2.52	0.45
1:C:35:VAL:N	1:C:36:PRO:HD2	2.32	0.45
1:C:27:THR:O	1:C:28:PRO:C	2.55	0.45
1:D:63:THR:OG1	1:D:67:LEU:HB3	2.16	0.45
1:A:276:ILE:O	1:A:298:ARG:NH1	2.49	0.45
1:B:281:MSE:HE3	1:B:283:THR:HG23	1.99	0.45
1:F:453:ARG:O	1:F:457:ARG:HG3	2.16	0.45
1:A:186:PRO:HG2	1:A:194:ILE:CG2	2.47	0.45
1:B:79:PHE:C	1:B:79:PHE:CD1	2.90	0.45
1:E:37:ALA:O	1:E:41:LYS:HG2	2.17	0.45
1:D:435:ASN:ND2	1:D:438:GLU:CG	2.79	0.45
1:A:361:ASN:C	1:A:362:ILE:HD12	2.38	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:145:LEU:HB3	1:F:146:PRO:CD	2.47	0.45
1:C:83:TYR:CZ	1:C:374:ASN:HB3	2.52	0.45
1:C:467:GLN:H	1:D:94:ASN:ND2	2.15	0.44
1:F:318:TYR:HA	1:F:321:LEU:HD13	1.98	0.44
1:A:287:GLN:NE2	1:A:290:VAL:HG23	2.32	0.44
1:D:26:PHE:CE1	1:D:61:ALA:HB2	2.52	0.44
1:B:221:PHE:CE1	1:B:223:PRO:HB3	2.52	0.44
1:E:256:GLN:HG3	1:E:382:PHE:CE1	2.52	0.44
1:B:271:GLY:HA2	1:B:298:ARG:CD	2.47	0.44
1:F:486:GLY:N	3:F:531:HOH:O	2.50	0.44
1:B:287:GLN:NE2	1:B:290:VAL:HG23	2.32	0.44
1:E:138:PRO:HG3	1:E:145:LEU:HD21	1.98	0.44
1:D:67:LEU:O	1:D:71:LEU:HB2	2.17	0.44
1:A:37:ALA:O	1:A:41:LYS:HG2	2.18	0.44
1:F:189:THR:HG23	1:F:190:PRO:HD2	2.00	0.44
1:F:252:PHE:O	1:F:253:LEU:HD13	2.17	0.44
1:D:221:PHE:CE1	1:D:223:PRO:HD3	2.52	0.44
1:A:79:PHE:C	1:A:79:PHE:CD1	2.91	0.44
1:D:37:ALA:O	1:D:41:LYS:HG2	2.17	0.44
1:D:242:GLU:OE2	1:D:247:ARG:NH2	2.50	0.44
1:A:284:GLU:HG3	1:A:382:PHE:CE2	2.52	0.44
1:C:453:ARG:O	1:C:457:ARG:HG3	2.17	0.44
1:F:284:GLU:HG3	1:F:382:PHE:CE2	2.53	0.44
1:A:27:THR:HA	1:A:62:SER:OG	2.17	0.44
1:E:287:GLN:NE2	1:E:290:VAL:HG23	2.32	0.44
1:A:357:ASP:HA	1:A:406:VAL:O	2.18	0.44
1:F:227:VAL:HG11	1:F:394:PRO:HB3	2.00	0.44
1:E:189:THR:HG23	1:E:190:PRO:HD2	2.00	0.44
1:F:439:ARG:O	1:F:443:ILE:HG13	2.18	0.44
1:D:357:ASP:OD2	1:D:361:ASN:HB2	2.18	0.44
1:E:397:MSE:HE3	3:E:560:HOH:O	2.17	0.44
1:B:283:THR:HB	1:B:284:GLU:H	1.70	0.44
1:E:63:THR:HB	1:E:67:LEU:HG	2.00	0.44
1:A:321:LEU:O	1:A:325:LYS:HB2	2.18	0.44
1:F:27:THR:O	1:F:31:ASN:ND2	2.51	0.44
1:B:221:PHE:CE1	1:B:223:PRO:HD3	2.52	0.44
1:E:89:LEU:O	1:E:93:ILE:HG13	2.18	0.44
1:B:131:THR:HG22	1:B:133:ASP:H	1.83	0.44
1:F:92:LEU:CD1	1:F:97:SER:HB2	2.47	0.44
1:F:22:GLY:HA2	1:F:58:PHE:O	2.18	0.44
1:A:179:PRO:HG2	1:B:387:TYR:HE2	1.83	0.43
1:B:397:MSE:HG2	1:B:398:LYS:N	2.32	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:257:SER:H	1:E:283:THR:CG2	2.31	0.43
1:F:276:ILE:O	1:F:298:ARG:NH1	2.51	0.43
1:B:435:ASN:HD21	1:B:438:GLU:CG	2.27	0.43
1:C:63:THR:HB	1:C:67:LEU:HG	1.98	0.43
1:B:252:PHE:HB2	1:B:277:PRO:HG2	2.00	0.43
1:B:83:TYR:CZ	1:B:374:ASN:HB3	2.53	0.43
1:B:293:LEU:O	1:B:298:ARG:HB3	2.18	0.43
1:F:252:PHE:HB2	1:F:277:PRO:HG2	2.01	0.43
1:A:357:ASP:N	3:A:536:HOH:O	2.51	0.43
1:E:357:ASP:HA	1:E:406:VAL:O	2.19	0.43
1:B:27:THR:O	1:B:28:PRO:C	2.56	0.43
1:B:257:SER:H	1:B:283:THR:CG2	2.30	0.43
1:F:331:ARG:CZ	3:F:527:HOH:O	2.66	0.43
1:D:256:GLN:CA	1:D:283:THR:HG22	2.46	0.43
1:C:321:LEU:O	1:C:325:LYS:HB2	2.18	0.43
1:B:189:THR:HG23	1:B:190:PRO:HD2	2.00	0.43
1:B:131:THR:HG21	1:B:133:ASP:OD1	2.17	0.43
1:D:92:LEU:CD1	1:D:97:SER:HB2	2.48	0.43
1:C:356:ALA:O	1:C:405:PHE:HA	2.19	0.43
1:C:242:GLU:OE2	1:C:247:ARG:NH2	2.51	0.43
1:A:27:THR:O	1:A:28:PRO:C	2.57	0.43
1:C:27:THR:HA	1:C:62:SER:OG	2.18	0.43
1:C:318:TYR:HA	1:C:321:LEU:HD13	2.00	0.43
1:D:189:THR:HG23	1:D:190:PRO:HD2	2.01	0.43
1:A:83:TYR:CZ	1:A:374:ASN:HB3	2.53	0.43
1:D:236:ALA:O	1:D:240:VAL:HG13	2.19	0.43
1:F:242:GLU:OE2	1:F:247:ARG:NH2	2.51	0.43
1:A:435:ASN:ND2	1:A:438:GLU:CG	2.81	0.43
1:D:439:ARG:O	1:D:443:ILE:HG13	2.18	0.43
1:A:145:LEU:HB3	1:A:146:PRO:CD	2.49	0.43
1:F:280:ASN:HD22	1:F:301:PHE:HB3	1.82	0.43
1:E:173:LEU:O	1:E:174:CYS:HB3	2.19	0.43
1:E:338:ASN:HA	1:E:339:PRO:HD3	1.91	0.43
1:F:63:THR:HB	1:F:67:LEU:HG	2.00	0.43
1:C:145:LEU:HB3	1:C:146:PRO:CD	2.49	0.43
1:F:138:PRO:HG3	1:F:145:LEU:HD21	2.01	0.43
1:E:356:ALA:O	1:E:405:PHE:HA	2.18	0.43
1:F:361:ASN:C	1:F:362:ILE:HD12	2.38	0.43
1:B:284:GLU:HG3	1:B:382:PHE:CE2	2.53	0.43
1:C:284:GLU:HG3	1:C:382:PHE:CE2	2.54	0.43
1:F:27:THR:O	1:F:28:PRO:C	2.57	0.43
1:C:218:GLU:HG3	1:C:219:SER:H	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:468:THR:HA	1:C:469:PRO:HD3	1.84	0.43
1:B:242:GLU:OE2	1:B:247:ARG:NH2	2.51	0.43
1:A:89:LEU:O	1:A:93:ILE:HG13	2.19	0.43
1:E:284:GLU:HG3	1:E:382:PHE:CE2	2.54	0.43
1:C:444:ILE:HA	1:C:448:VAL:CG2	2.48	0.43
1:C:276:ILE:O	1:C:298:ARG:NH1	2.52	0.43
1:C:439:ARG:O	1:C:443:ILE:HG13	2.18	0.43
1:C:387:TYR:CE2	1:D:179:PRO:HG2	2.52	0.43
1:F:359:PHE:CE2	1:F:469:PRO:HD2	2.53	0.43
1:E:357:ASP:OD2	1:E:361:ASN:HB2	2.18	0.43
1:E:397:MSE:HG2	1:E:398:LYS:N	2.34	0.43
1:C:467:GLN:N	1:D:94:ASN:HD22	2.14	0.43
1:C:283:THR:HB	1:C:284:GLU:H	1.68	0.43
1:A:453:ARG:O	1:A:457:ARG:HG3	2.19	0.43
1:E:167:ILE:HD13	1:E:167:ILE:HA	1.84	0.43
1:E:145:LEU:HB3	1:E:146:PRO:CD	2.49	0.43
1:D:227:VAL:HG11	1:D:394:PRO:HB3	2.01	0.43
1:E:227:VAL:HG11	1:E:394:PRO:HB3	2.01	0.43
1:F:409:VAL:HG23	1:F:412:HIS:CD2	2.54	0.42
1:A:356:ALA:O	1:A:405:PHE:HA	2.19	0.42
1:F:397:MSE:HB3	1:F:402:ILE:HB	2.01	0.42
1:B:468:THR:HA	1:B:469:PRO:HD3	1.83	0.42
1:A:403:SER:H	1:A:488:MSE:SE	2.52	0.42
1:D:293:LEU:O	1:D:298:ARG:HB3	2.19	0.42
1:C:355:GLU:HG3	1:C:409:VAL:HG12	2.01	0.42
1:B:92:LEU:CD1	1:B:97:SER:HB2	2.49	0.42
1:F:184:GLU:O	1:F:186:PRO:HD3	2.19	0.42
1:E:136:ILE:N	1:E:136:ILE:HD12	2.34	0.42
1:E:361:ASN:C	1:E:362:ILE:HD12	2.40	0.42
1:E:92:LEU:CD1	1:E:97:SER:HB2	2.49	0.42
1:A:242:GLU:OE2	1:A:247:ARG:NH2	2.52	0.42
1:A:252:PHE:HB2	1:A:277:PRO:HG2	2.01	0.42
1:D:94:ASN:ND2	1:D:372:MSE:H	2.01	0.42
1:B:63:THR:HB	1:B:67:LEU:HG	2.02	0.42
1:F:341:ILE:N	1:F:341:ILE:HD13	2.34	0.42
1:F:444:ILE:HA	1:F:448:VAL:CG2	2.50	0.42
1:E:166:GLU:O	1:E:325:LYS:HE2	2.19	0.42
1:B:357:ASP:OD2	1:B:361:ASN:HB2	2.19	0.42
1:D:22:GLY:HA2	1:D:58:PHE:O	2.20	0.42
1:D:293:LEU:HD22	1:D:298:ARG:CG	2.45	0.42
1:A:318:TYR:HA	1:A:321:LEU:HD13	2.00	0.42
1:B:318:TYR:HA	1:B:321:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:468:THR:HA	1:F:469:PRO:HD3	1.82	0.42
1:B:487:ASP:HB3	1:B:490:ASN:ND2	2.35	0.42
1:F:240:VAL:CG2	3:F:511:HOH:O	2.67	0.42
1:C:138:PRO:HG3	1:C:145:LEU:HD21	2.00	0.42
1:C:221:PHE:CE1	1:C:223:PRO:HB3	2.54	0.42
1:C:236:ALA:O	1:C:240:VAL:HG13	2.18	0.42
1:D:409:VAL:HG23	1:D:412:HIS:CD2	2.54	0.42
1:D:267:LEU:O	1:D:293:LEU:HD11	2.20	0.42
1:E:409:VAL:HG23	1:E:412:HIS:CD2	2.54	0.42
1:D:318:TYR:HA	1:D:321:LEU:HD13	2.01	0.42
1:D:287:GLN:NE2	1:D:290:VAL:HG23	2.35	0.42
1:D:357:ASP:HA	1:D:406:VAL:O	2.20	0.42
1:F:83:TYR:CZ	1:F:374:ASN:HB3	2.54	0.42
1:C:252:PHE:HB2	1:C:277:PRO:HG2	2.02	0.42
1:C:37:ALA:O	1:C:41:LYS:HG2	2.19	0.42
1:C:79:PHE:CD1	1:C:79:PHE:C	2.92	0.42
1:D:354:LEU:HD11	1:D:373:MSE:HG3	2.02	0.42
1:C:218:GLU:CG	1:C:219:SER:N	2.83	0.42
1:F:236:ALA:O	1:F:240:VAL:HG13	2.19	0.42
1:B:356:ALA:O	1:B:405:PHE:HA	2.20	0.42
1:A:221:PHE:CE1	1:A:223:PRO:HB3	2.54	0.42
1:A:127:VAL:HG12	1:A:128:ALA:N	2.35	0.42
1:B:158:GLU:OE1	3:B:513:HOH:O	2.21	0.42
1:A:236:ALA:O	1:A:240:VAL:HG13	2.19	0.42
1:A:293:LEU:HD22	1:A:298:ARG:CG	2.45	0.42
1:E:318:TYR:HA	1:E:321:LEU:HD13	2.01	0.42
1:E:437:ARG:NE	3:E:533:HOH:O	2.30	0.42
1:A:63:THR:HB	1:A:67:LEU:HG	2.01	0.42
1:D:221:PHE:CE1	1:D:223:PRO:HB3	2.54	0.42
1:B:54:LYS:HG2	1:B:76:ALA:HA	2.01	0.41
1:C:435:ASN:ND2	1:C:438:GLU:CG	2.83	0.41
1:C:163:HIS:HA	1:C:164:PRO:HD2	1.94	0.41
1:A:67:LEU:HB3	1:A:68:ASP:H	1.77	0.41
1:E:288:ASP:HB2	3:E:510:HOH:O	2.20	0.41
1:C:357:ASP:HA	1:C:406:VAL:O	2.19	0.41
1:A:444:ILE:HA	1:A:448:VAL:CG2	2.50	0.41
1:F:293:LEU:HD22	1:F:298:ARG:CG	2.46	0.41
1:D:453:ARG:O	1:D:457:ARG:HG3	2.20	0.41
1:D:167:ILE:HD13	1:D:167:ILE:HA	1.85	0.41
1:F:280:ASN:ND2	1:F:300:LYS:HB2	2.34	0.41
1:D:138:PRO:HG3	1:D:145:LEU:HD21	2.00	0.41
1:F:221:PHE:CZ	1:F:223:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:221:PHE:CZ	1:D:223:PRO:HG3	2.55	0.41
1:A:221:PHE:CE1	1:A:223:PRO:HD3	2.55	0.41
1:E:387:TYR:HD1	1:E:388:VAL:HG23	1.85	0.41
1:D:83:TYR:CZ	1:D:374:ASN:HB3	2.56	0.41
1:F:357:ASP:HA	1:F:406:VAL:O	2.19	0.41
1:B:22:GLY:HA2	1:B:58:PHE:O	2.20	0.41
1:D:468:THR:HA	1:D:469:PRO:HD3	1.83	0.41
1:B:136:ILE:HD12	1:B:136:ILE:N	2.35	0.41
1:F:17:HIS:CD2	1:F:53:PHE:HA	2.55	0.41
1:D:163:HIS:HA	1:D:164:PRO:HD2	1.95	0.41
1:A:163:HIS:HA	1:A:164:PRO:HD2	1.92	0.41
1:B:186:PRO:HG2	1:B:194:ILE:CG2	2.51	0.41
1:C:409:VAL:HG23	1:C:412:HIS:CD2	2.55	0.41
1:F:131:THR:HG22	1:F:133:ASP:H	1.85	0.41
1:F:63:THR:OG1	1:F:67:LEU:HB3	2.20	0.41
1:E:184:GLU:O	1:E:186:PRO:HD3	2.20	0.41
1:A:221:PHE:CZ	1:A:223:PRO:HG3	2.55	0.41
1:E:83:TYR:CZ	1:E:374:ASN:HB3	2.55	0.41
1:F:54:LYS:HG2	1:F:76:ALA:HA	2.01	0.41
1:D:284:GLU:HG3	1:D:382:PHE:CE2	2.55	0.41
1:E:293:LEU:HD22	1:E:298:ARG:CG	2.43	0.41
1:E:63:THR:OG1	1:E:67:LEU:HB3	2.20	0.41
1:B:341:ILE:HD13	1:B:341:ILE:N	2.35	0.41
1:C:26:PHE:O	1:C:27:THR:HG23	2.21	0.41
1:A:355:GLU:HG3	1:A:409:VAL:HG12	2.02	0.41
1:B:354:LEU:HD11	1:B:373:MSE:HG3	2.03	0.41
1:E:293:LEU:O	1:E:298:ARG:HB3	2.20	0.41
1:B:184:GLU:O	1:B:186:PRO:HD3	2.21	0.41
1:B:145:LEU:HB3	1:B:146:PRO:CD	2.51	0.41
1:B:138:PRO:HG3	1:B:145:LEU:HD21	2.02	0.41
1:B:227:VAL:HG11	1:B:394:PRO:HB3	2.03	0.41
1:F:407:PRO:HD2	3:F:538:HOH:O	2.20	0.41
1:C:26:PHE:C	1:C:27:THR:HG23	2.40	0.41
1:D:252:PHE:HB2	1:D:277:PRO:HG2	2.02	0.41
1:F:131:THR:HG21	1:F:133:ASP:OD1	2.21	0.41
1:B:221:PHE:CD1	1:B:223:PRO:HD3	2.56	0.41
1:D:221:PHE:CD1	1:D:223:PRO:HD3	2.56	0.41
1:A:221:PHE:CD1	1:A:223:PRO:HD3	2.56	0.41
1:D:356:ALA:O	1:D:405:PHE:HA	2.20	0.41
1:F:356:ALA:O	1:F:405:PHE:HA	2.20	0.41
1:F:136:ILE:HD12	1:F:136:ILE:N	2.35	0.41
1:E:127:VAL:HG12	1:E:128:ALA:N	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:26:PHE:O	1:F:27:THR:HG23	2.21	0.41
1:E:252:PHE:O	1:E:253:LEU:HD13	2.21	0.41
1:D:252:PHE:O	1:D:253:LEU:HD13	2.21	0.41
1:D:131:THR:HG22	1:D:133:ASP:H	1.86	0.41
1:D:131:THR:HG21	1:D:133:ASP:OD1	2.18	0.41
1:D:184:GLU:O	1:D:186:PRO:HD3	2.21	0.41
1:F:221:PHE:CD1	1:F:223:PRO:HD3	2.55	0.41
1:F:239:LEU:HA	1:F:239:LEU:HD12	1.84	0.41
1:E:256:GLN:CA	1:E:283:THR:HG22	2.45	0.41
1:D:102:ASP:OD2	1:D:102:ASP:N	2.51	0.41
1:F:167:ILE:HA	1:F:167:ILE:HD13	1.84	0.41
1:A:284:GLU:HG3	1:A:382:PHE:HE2	1.86	0.40
1:E:163:HIS:HA	1:E:164:PRO:HD2	1.93	0.40
1:A:218:GLU:HG3	1:A:219:SER:H	1.85	0.40
1:D:145:LEU:HB3	1:D:146:PRO:CD	2.51	0.40
1:B:221:PHE:CZ	1:B:223:PRO:HG3	2.56	0.40
1:E:468:THR:HA	1:E:469:PRO:HD3	1.85	0.40
1:C:147:THR:HG22	1:C:151:LEU:HD22	2.03	0.40
1:E:22:GLY:HA2	1:E:58:PHE:O	2.21	0.40
1:A:267:LEU:O	1:A:293:LEU:HD11	2.21	0.40
1:E:257:SER:HA	1:E:350:ILE:O	2.21	0.40
1:E:267:LEU:O	1:E:293:LEU:HD11	2.21	0.40
1:F:283:THR:HB	1:F:284:GLU:H	1.69	0.40
1:B:409:VAL:HG23	1:B:412:HIS:CD2	2.56	0.40
1:B:26:PHE:CE1	1:B:61:ALA:HB2	2.55	0.40
1:A:409:VAL:HG23	1:A:412:HIS:CD2	2.57	0.40
1:E:439:ARG:O	1:E:443:ILE:HG13	2.21	0.40
1:A:138:PRO:HG3	1:A:145:LEU:HD21	2.02	0.40
1:E:231:ILE:O	1:E:235:VAL:HG23	2.21	0.40
1:E:242:GLU:OE2	1:E:247:ARG:NH2	2.54	0.40
1:E:54:LYS:HG2	1:E:76:ALA:HA	2.02	0.40
1:C:294:MSE:CE	1:C:324:PHE:CD2	3.04	0.40
1:A:189:THR:HG23	1:A:190:PRO:HD2	2.04	0.40
1:F:35:VAL:O	1:F:39:ILE:HG12	2.22	0.40
1:B:403:SER:H	1:B:488:MSE:SE	2.55	0.40
1:A:124:ILE:CD1	1:A:156:ILE:HD12	2.51	0.40
1:C:284:GLU:HG3	1:C:382:PHE:HE2	1.85	0.40
1:F:453:ARG:CD	3:F:515:HOH:O	2.69	0.40
1:F:378:GLY:O	1:F:382:PHE:HD2	2.04	0.40
1:F:267:LEU:O	1:F:293:LEU:HD11	2.21	0.40
1:A:26:PHE:C	1:A:27:THR:HG23	2.42	0.40
1:A:131:THR:HG22	1:A:133:ASP:H	1.85	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:92:LEU:HB2	3:E:539:HOH:O	2.20	0.40
1:A:22:GLY:HA2	1:A:58:PHE:O	2.21	0.40
1:D:408:MSE:HG3	3:D:518:HOH:O	2.22	0.40
1:E:78:LYS:HE3	1:E:78:LYS:HB2	1.95	0.40
1:B:357:ASP:HA	1:B:406:VAL:O	2.21	0.40
1:E:131:THR:HG21	1:E:133:ASP:OD1	2.22	0.40
1:C:221:PHE:CE1	1:C:223:PRO:HD3	2.55	0.40
1:C:227:VAL:HG11	1:C:394:PRO:HB3	2.03	0.40
1:B:124:ILE:CD1	1:B:156:ILE:HD12	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/506 (98%)	458 (93%)	33 (7%)	3 (1%)	33	66
1	B	494/506 (98%)	462 (94%)	29 (6%)	3 (1%)	33	66
1	C	494/506 (98%)	460 (93%)	31 (6%)	3 (1%)	33	66
1	D	494/506 (98%)	461 (93%)	29 (6%)	4 (1%)	27	58
1	E	494/506 (98%)	461 (93%)	29 (6%)	4 (1%)	27	58
1	F	494/506 (98%)	460 (93%)	30 (6%)	4 (1%)	27	58
All	All	2964/3036 (98%)	2762 (93%)	181 (6%)	21 (1%)	30	62

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	GLY
1	A	221	PHE
1	B	118	GLY
1	B	221	PHE
1	C	118	GLY
1	C	221	PHE

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Mol	Chain	Res	Type
1	D	118	GLY
1	D	221	PHE
1	E	118	GLY
1	E	221	PHE
1	F	118	GLY
1	F	221	PHE
1	A	186	PRO
1	E	186	PRO
1	B	186	PRO
1	C	186	PRO
1	D	186	PRO
1	F	186	PRO
1	E	27	THR
1	F	27	THR
1	D	27	THR

### 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	416/413 (101%)	398 (96%)	18 (4%)	40	72
1	B	416/413 (101%)	398 (96%)	18 (4%)	40	72
1	C	416/413 (101%)	397 (95%)	19 (5%)	37	70
1	D	416/413 (101%)	397 (95%)	19 (5%)	37	70
1	E	416/413 (101%)	398 (96%)	18 (4%)	40	72
1	F	416/413 (101%)	398 (96%)	18 (4%)	40	72
All	All	2496/2478 (101%)	2386 (96%)	110 (4%)	39	71

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	71	LEU
1	A	81	THR
1	A	122	VAL

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Mol	Chain	Res	Type
1	A	151	LEU
1	A	159	LEU
1	A	161	ASP
1	A	177	LEU
1	A	199	VAL
1	A	239	LEU
1	A	252	PHE
1	A	253	LEU
1	A	287	GLN
1	A	322	ASP
1	A	373	MSE
1	A	431	LEU
1	A	435	ASN
1	A	467	GLN
1	B	67	LEU
1	B	71	LEU
1	B	81	THR
1	B	122	VAL
1	B	151	LEU
1	B	159	LEU
1	B	161	ASP
1	B	177	LEU
1	B	199	VAL
1	B	239	LEU
1	B	252	PHE
1	B	253	LEU
1	B	287	GLN
1	B	322	ASP
1	B	373	MSE
1	B	431	LEU
1	B	435	ASN
1	B	467	GLN
1	C	67	LEU
1	C	71	LEU
1	C	81	THR
1	C	122	VAL
1	C	150	ARG
1	C	151	LEU
1	C	159	LEU
1	C	161	ASP
1	C	177	LEU
1	C	199	VAL

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Mol	Chain	Res	Type
1	C	239	LEU
1	C	252	PHE
1	C	253	LEU
1	C	287	GLN
1	C	322	ASP
1	C	373	MSE
1	C	431	LEU
1	C	435	ASN
1	C	467	GLN
1	D	67	LEU
1	D	71	LEU
1	D	81	THR
1	D	122	VAL
1	D	150	ARG
1	D	151	LEU
1	D	159	LEU
1	D	161	ASP
1	D	177	LEU
1	D	199	VAL
1	D	239	LEU
1	D	252	PHE
1	D	253	LEU
1	D	287	GLN
1	D	322	ASP
1	D	373	MSE
1	D	431	LEU
1	D	435	ASN
1	D	467	GLN
1	E	67	LEU
1	E	71	LEU
1	E	81	THR
1	E	122	VAL
1	E	151	LEU
1	E	159	LEU
1	E	161	ASP
1	E	177	LEU
1	E	199	VAL
1	E	239	LEU
1	E	252	PHE
1	E	253	LEU
1	E	287	GLN
1	E	322	ASP

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Mol	Chain	Res	Type
1	E	373	MSE
1	E	431	LEU
1	E	435	ASN
1	E	467	GLN
1	F	67	LEU
1	F	71	LEU
1	F	81	THR
1	F	122	VAL
1	F	151	LEU
1	F	159	LEU
1	F	161	ASP
1	F	177	LEU
1	F	199	VAL
1	F	239	LEU
1	F	252	PHE
1	F	253	LEU
1	F	287	GLN
1	F	322	ASP
1	F	373	MSE
1	F	431	LEU
1	F	435	ASN
1	F	467	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	51	ASN
1	A	91	ASN
1	A	94	ASN
1	A	95	ASN
1	A	104	HIS
1	A	163	HIS
1	A	261	ASN
1	A	264	ASN
1	A	280	ASN
1	A	287	GLN
1	A	374	ASN
1	A	412	HIS
1	A	435	ASN
1	A	467	GLN
1	A	479	HIS

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Mol	Chain	Res	Type
1	A	480	GLN
1	A	490	ASN
1	B	17	HIS
1	B	51	ASN
1	B	91	ASN
1	B	94	ASN
1	B	95	ASN
1	B	163	HIS
1	B	261	ASN
1	B	264	ASN
1	B	280	ASN
1	B	287	GLN
1	B	374	ASN
1	B	412	HIS
1	B	435	ASN
1	B	441	HIS
1	B	467	GLN
1	B	480	GLN
1	B	490	ASN
1	C	17	HIS
1	C	51	ASN
1	C	91	ASN
1	C	94	ASN
1	C	95	ASN
1	C	163	HIS
1	C	261	ASN
1	C	264	ASN
1	C	280	ASN
1	C	287	GLN
1	C	374	ASN
1	C	412	HIS
1	C	435	ASN
1	C	441	HIS
1	C	467	GLN
1	C	479	HIS
1	C	480	GLN
1	C	490	ASN
1	D	17	HIS
1	D	47	HIS
1	D	51	ASN
1	D	91	ASN
1	D	94	ASN

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Mol	Chain	Res	Type
1	D	95	ASN
1	D	163	HIS
1	D	261	ASN
1	D	264	ASN
1	D	280	ASN
1	D	287	GLN
1	D	374	ASN
1	D	412	HIS
1	D	435	ASN
1	D	467	GLN
1	D	479	HIS
1	D	480	GLN
1	D	490	ASN
1	E	17	HIS
1	E	47	HIS
1	E	51	ASN
1	E	91	ASN
1	E	94	ASN
1	E	95	ASN
1	E	163	HIS
1	E	216	ASN
1	E	261	ASN
1	E	264	ASN
1	E	280	ASN
1	E	287	GLN
1	E	374	ASN
1	E	412	HIS
1	E	414	HIS
1	E	435	ASN
1	E	467	GLN
1	E	479	HIS
1	E	480	GLN
1	E	490	ASN
1	F	17	HIS
1	F	47	HIS
1	F	51	ASN
1	F	91	ASN
1	F	94	ASN
1	F	95	ASN
1	F	163	HIS
1	F	261	ASN
1	F	264	ASN

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Mol	Chain	Res	Type
1	F	280	ASN
1	F	287	GLN
1	F	374	ASN
1	F	412	HIS
1	F	435	ASN
1	F	467	GLN
1	F	479	HIS
1	F	480	GLN
1	F	490	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	496/506 (98%)	1.81	175 (35%) 1 1	6, 7, 19, 40	0
1	B	496/506 (98%)	1.90	202 (40%) 1 0	6, 7, 19, 40	0
1	C	496/506 (98%)	1.82	178 (35%) 1 1	6, 7, 19, 40	0
1	D	496/506 (98%)	1.99	201 (40%) 1 0	6, 7, 19, 40	0
1	E	496/506 (98%)	2.64	332 (66%) 0 0	6, 7, 19, 40	0
1	F	496/506 (98%)	2.70	323 (65%) 0 0	6, 7, 19, 40	0
All	All	2976/3036 (98%)	2.14	1411 (47%) 1 0	6, 7, 19, 40	0

All (1411) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	427	GLY	8.9
1	F	232	GLY	8.2
1	F	57	MSE	7.8
1	F	134	GLY	7.5
1	C	85	SER	7.1
1	F	299	ILE	7.0
1	F	290	VAL	6.8
1	E	393	THR	6.8
1	E	405	PHE	6.8
1	F	227	VAL	6.5
1	E	60	GLY	6.5
1	E	365	THR	6.4
1	F	149	CYS	6.4
1	E	383	THR	6.2
1	E	345	LEU	6.2
1	F	170	MSE	6.1
1	F	99	SER	6.1
1	B	373	MSE	6.0
1	E	318	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	326	ASP	5.9
1	E	116	PHE	5.9
1	E	447	CYS	5.9
1	F	199	VAL	5.8
1	F	58	PHE	5.8
1	F	127	VAL	5.8
1	E	483	ALA	5.7
1	D	207	VAL	5.7
1	F	449	HIS	5.7
1	D	220	ASP	5.6
1	E	222	ALA	5.6
1	F	229	GLN	5.6
1	F	168	MSE	5.6
1	F	407	PRO	5.6
1	D	55	ILE	5.6
1	F	138	PRO	5.5
1	F	497	MSE	5.5
1	D	410	ALA	5.5
1	A	222	ALA	5.4
1	E	85	SER	5.4
1	F	328	ILE	5.4
1	E	157	VAL	5.4
1	F	130	VAL	5.4
1	F	136	ILE	5.4
1	F	494	GLU	5.4
1	F	447	CYS	5.4
1	B	122	VAL	5.3
1	A	221	PHE	5.3
1	F	221	PHE	5.3
1	E	217	ASP	5.3
1	F	478	PHE	5.3
1	E	370	THR	5.3
1	F	230	ALA	5.3
1	F	270	LEU	5.3
1	E	125	ILE	5.3
1	F	190	PRO	5.2
1	F	462	LEU	5.2
1	F	11	ALA	5.2
1	F	201	VAL	5.2
1	D	354	LEU	5.2
1	F	223	PRO	5.2
1	F	493	TRP	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	116	PHE	5.2
1	D	221	PHE	5.2
1	D	307	LEU	5.2
1	F	382	PHE	5.1
1	F	350	ILE	5.1
1	F	376	ILE	5.1
1	E	352	THR	5.1
1	F	123	ALA	5.1
1	E	89	LEU	5.1
1	E	223	PRO	5.1
1	E	203	PRO	5.1
1	F	467	GLN	5.1
1	F	374	ASN	5.1
1	D	118	GLY	5.1
1	A	125	ILE	5.1
1	E	363	ASN	5.1
1	E	432	ARG	5.1
1	D	352	THR	5.0
1	C	350	ILE	5.0
1	E	33	LYS	5.0
1	F	359	PHE	5.0
1	B	99	SER	5.0
1	E	259	VAL	5.0
1	E	376	ILE	4.9
1	E	477	ALA	4.9
1	F	248	ILE	4.9
1	F	50	GLY	4.9
1	F	318	TYR	4.9
1	D	63	THR	4.9
1	C	376	ILE	4.9
1	F	361	ASN	4.9
1	E	52	PRO	4.8
1	F	208	GLY	4.8
1	B	255	LEU	4.8
1	A	373	MSE	4.8
1	A	398	LYS	4.8
1	E	328	ILE	4.8
1	E	12	ALA	4.8
1	E	322	ASP	4.7
1	D	137	LEU	4.7
1	E	410	ALA	4.7
1	F	255	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	496	TYR	4.7
1	F	291	ILE	4.7
1	D	241	SER	4.7
1	F	383	THR	4.7
1	E	159	LEU	4.6
1	F	472	LEU	4.6
1	A	40	ALA	4.6
1	F	274	PRO	4.6
1	F	286	ILE	4.6
1	E	221	PHE	4.6
1	F	409	VAL	4.6
1	E	497	MSE	4.6
1	E	307	LEU	4.6
1	C	219	SER	4.6
1	E	14	PHE	4.6
1	E	388	VAL	4.6
1	D	147	THR	4.6
1	B	43	ALA	4.6
1	B	400	GLY	4.6
1	E	185	LEU	4.6
1	F	185	LEU	4.6
1	B	221	PHE	4.6
1	E	119	LYS	4.5
1	E	353	ALA	4.5
1	F	148	ILE	4.5
1	F	59	THR	4.5
1	F	68	ASP	4.5
1	E	81	THR	4.5
1	F	282	TYR	4.5
1	C	374	ASN	4.5
1	A	21	VAL	4.5
1	F	408	MSE	4.5
1	F	257	SER	4.5
1	B	231	ILE	4.5
1	A	34	VAL	4.5
1	D	318	TYR	4.5
1	F	323	PHE	4.5
1	D	167	ILE	4.5
1	D	315	GLN	4.5
1	E	428	VAL	4.5
1	E	178	ASP	4.5
1	F	263	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	285	VAL	4.4
1	E	464	VAL	4.4
1	E	360	GLY	4.4
1	C	496	TYR	4.4
1	B	8	ALA	4.4
1	F	124	ILE	4.4
1	F	426	TRP	4.4
1	F	276	ILE	4.4
1	E	209	VAL	4.4
1	E	379	SER	4.4
1	F	238	PHE	4.4
1	F	289	ALA	4.4
1	D	327	LYS	4.4
1	E	354	LEU	4.3
1	F	117	TYR	4.3
1	E	77	VAL	4.3
1	D	112	LEU	4.3
1	F	325	LYS	4.3
1	E	204	ALA	4.3
1	B	452	TYR	4.3
1	F	491	VAL	4.3
1	F	63	THR	4.3
1	F	209	VAL	4.3
1	B	112	LEU	4.3
1	F	72	ALA	4.3
1	F	402	ILE	4.3
1	A	117	TYR	4.3
1	E	309	VAL	4.3
1	F	207	VAL	4.3
1	E	143	GLY	4.3
1	F	326	ASP	4.2
1	F	112	LEU	4.2
1	B	2	ALA	4.2
1	D	21	VAL	4.2
1	D	322	ASP	4.2
1	F	193	ARG	4.2
1	D	449	HIS	4.2
1	E	319	ALA	4.2
1	B	497	MSE	4.2
1	C	63	THR	4.2
1	D	349	THR	4.2
1	E	492	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	173	LEU	4.2
1	E	240	VAL	4.2
1	A	186	PRO	4.2
1	E	373	MSE	4.2
1	F	85	SER	4.2
1	E	278	ALA	4.2
1	B	7	THR	4.2
1	E	418	SER	4.2
1	A	64	GLY	4.2
1	F	475	CYS	4.2
1	D	156	ILE	4.2
1	E	151	LEU	4.2
1	E	337	ASN	4.1
1	A	173	LEU	4.1
1	F	330	LEU	4.1
1	E	144	ILE	4.1
1	C	32	PRO	4.1
1	B	3	LEU	4.1
1	E	21	VAL	4.1
1	F	410	ALA	4.1
1	B	397	MSE	4.1
1	D	32	PRO	4.1
1	E	42	ARG	4.1
1	F	264	ASN	4.1
1	A	477	ALA	4.1
1	D	136	ILE	4.1
1	F	194	ILE	4.1
1	F	351	ASN	4.1
1	F	188	TYR	4.1
1	B	448	VAL	4.1
1	C	99	SER	4.1
1	E	224	LEU	4.1
1	D	18	ASN	4.0
1	D	491	VAL	4.0
1	A	2	ALA	4.0
1	F	30	GLY	4.0
1	D	146	PRO	4.0
1	C	352	THR	4.0
1	E	118	GLY	4.0
1	F	107	THR	4.0
1	F	269	ALA	4.0
1	C	93	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	122	VAL	4.0
1	E	2	ALA	4.0
1	A	497	MSE	4.0
1	A	339	PRO	4.0
1	B	326	ASP	4.0
1	C	133	ASP	4.0
1	F	77	VAL	4.0
1	A	7	THR	4.0
1	E	422	ILE	4.0
1	F	329	LEU	4.0
1	E	361	ASN	4.0
1	E	102	ASP	3.9
1	D	373	MSE	3.9
1	E	423	ILE	3.9
1	E	415	SER	3.9
1	A	197	PRO	3.9
1	E	17	HIS	3.9
1	B	370	THR	3.9
1	B	58	PHE	3.9
1	D	431	LEU	3.9
1	D	317	ILE	3.9
1	D	350	ILE	3.9
1	D	388	VAL	3.9
1	D	497	MSE	3.9
1	F	327	LYS	3.9
1	F	284	GLU	3.9
1	E	296	LYS	3.9
1	C	28	PRO	3.9
1	C	136	ILE	3.9
1	F	44	ILE	3.9
1	D	365	THR	3.9
1	A	99	SER	3.9
1	E	26	PHE	3.9
1	E	75	ASP	3.9
1	E	255	LEU	3.9
1	E	142	VAL	3.8
1	D	393	THR	3.8
1	F	105	LEU	3.8
1	F	133	ASP	3.8
1	E	79	PHE	3.8
1	E	375	GLY	3.8
1	E	37	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	128	ALA	3.8
1	F	373	MSE	3.8
1	E	340	GLU	3.8
1	C	349	THR	3.8
1	D	170	MSE	3.8
1	D	219	SER	3.8
1	E	212	THR	3.8
1	C	223	PRO	3.8
1	B	286	ILE	3.8
1	E	349	THR	3.8
1	D	26	PHE	3.8
1	F	8	ALA	3.8
1	F	300	LYS	3.8
1	A	452	TYR	3.8
1	A	187	VAL	3.8
1	C	403	SER	3.8
1	D	383	THR	3.8
1	E	286	ILE	3.8
1	E	245	ALA	3.8
1	E	389	SER	3.7
1	F	429	ALA	3.7
1	F	161	ASP	3.7
1	F	412	HIS	3.7
1	F	464	VAL	3.7
1	E	98	THR	3.7
1	E	66	ARG	3.7
1	E	164	PRO	3.7
1	E	411	HIS	3.7
1	B	64	GLY	3.7
1	B	342	VAL	3.7
1	B	210	VAL	3.7
1	E	120	VAL	3.7
1	E	108	LEU	3.7
1	F	252	PHE	3.7
1	D	102	ASP	3.7
1	A	195	GLY	3.7
1	E	27	THR	3.7
1	F	155	ILE	3.7
1	F	370	THR	3.7
1	F	324	PHE	3.7
1	A	369	GLY	3.7
1	B	447	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	156	ILE	3.7
1	C	360	GLY	3.7
1	F	389	SER	3.7
1	E	105	LEU	3.7
1	F	285	VAL	3.7
1	E	218	GLU	3.7
1	D	375	GLY	3.6
1	E	92	LEU	3.6
1	F	390	ILE	3.6
1	B	74	ALA	3.6
1	F	346	GLY	3.6
1	C	239	LEU	3.6
1	E	188	TYR	3.6
1	E	335	TYR	3.6
1	F	83	TYR	3.6
1	F	200	GLN	3.6
1	E	24	SER	3.6
1	A	122	VAL	3.6
1	E	150	ARG	3.6
1	F	228	THR	3.6
1	E	53	PHE	3.6
1	E	51	ASN	3.6
1	E	232	GLY	3.6
1	F	213	SER	3.6
1	F	283	THR	3.6
1	D	44	ILE	3.6
1	F	167	ILE	3.6
1	E	306	SER	3.6
1	E	6	ILE	3.6
1	D	403	SER	3.6
1	F	294	MSE	3.6
1	D	300	LYS	3.6
1	C	31	ASN	3.6
1	B	269	ALA	3.6
1	F	46	ALA	3.6
1	E	15	VAL	3.6
1	E	228	THR	3.6
1	F	26	PHE	3.6
1	E	16	HIS	3.5
1	E	61	ALA	3.5
1	B	36	PRO	3.5
1	C	10	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	177	LEU	3.5
1	E	438	GLU	3.5
1	E	31	ASN	3.5
1	F	147	THR	3.5
1	E	93	ILE	3.5
1	B	305	CYS	3.5
1	D	97	SER	3.5
1	E	28	PRO	3.5
1	D	68	ASP	3.5
1	E	192	ASP	3.5
1	A	120	VAL	3.5
1	E	216	ASN	3.5
1	F	398	LYS	3.5
1	C	156	ILE	3.5
1	E	469	PRO	3.5
1	F	340	GLU	3.5
1	A	455	LEU	3.5
1	D	37	ALA	3.5
1	B	398	LYS	3.5
1	F	452	TYR	3.5
1	A	67	LEU	3.5
1	F	187	VAL	3.5
1	F	179	PRO	3.5
1	A	443	ILE	3.5
1	F	417	HIS	3.5
1	B	218	GLU	3.5
1	E	20	ASN	3.5
1	E	199	VAL	3.5
1	A	131	THR	3.5
1	E	317	ILE	3.5
1	C	225	ASP	3.5
1	F	41	LYS	3.5
1	E	131	THR	3.5
1	F	334	GLU	3.4
1	A	108	LEU	3.4
1	D	239	LEU	3.4
1	B	186	PRO	3.4
1	D	164	PRO	3.4
1	C	127	VAL	3.4
1	D	77	VAL	3.4
1	E	266	VAL	3.4
1	B	394	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	348	ILE	3.4
1	D	208	GLY	3.4
1	E	350	ILE	3.4
1	E	491	VAL	3.4
1	E	272	ASP	3.4
1	E	263	ALA	3.4
1	E	402	ILE	3.4
1	D	4	ARG	3.4
1	E	95	ASN	3.4
1	E	183	ARG	3.4
1	F	321	LEU	3.4
1	E	308	SER	3.4
1	E	414	HIS	3.4
1	A	190	PRO	3.4
1	B	339	PRO	3.4
1	E	48	GLU	3.4
1	F	224	LEU	3.4
1	D	266	VAL	3.4
1	F	56	GLY	3.4
1	F	369	GLY	3.4
1	D	353	ALA	3.4
1	F	29	ALA	3.4
1	F	237	ALA	3.4
1	E	436	PRO	3.4
1	D	135	LYS	3.4
1	F	303	SER	3.4
1	D	262	VAL	3.4
1	C	447	CYS	3.3
1	F	36	PRO	3.3
1	F	490	ASN	3.3
1	B	139	THR	3.3
1	B	223	PRO	3.3
1	B	429	ALA	3.3
1	E	11	ALA	3.3
1	E	149	CYS	3.3
1	A	448	VAL	3.3
1	B	130	VAL	3.3
1	F	163	HIS	3.3
1	F	476	PHE	3.3
1	E	83	TYR	3.3
1	B	264	ASN	3.3
1	F	18	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	299	ILE	3.3
1	B	224	LEU	3.3
1	F	25	GLY	3.3
1	A	224	LEU	3.3
1	E	372	MSE	3.3
1	C	57	MSE	3.3
1	B	70	VAL	3.3
1	B	131	THR	3.3
1	B	419	VAL	3.3
1	C	259	VAL	3.3
1	C	166	GLU	3.3
1	D	274	PRO	3.3
1	A	89	LEU	3.3
1	E	248	ILE	3.3
1	F	93	ILE	3.3
1	E	310	SER	3.3
1	F	262	VAL	3.3
1	A	460	LEU	3.3
1	F	345	LEU	3.3
1	C	379	SER	3.3
1	B	372	MSE	3.2
1	F	320	ASN	3.2
1	F	385	ASN	3.2
1	E	189	THR	3.2
1	E	426	TRP	3.2
1	F	341	ILE	3.2
1	B	336	SER	3.2
1	A	234	ASN	3.2
1	C	26	PHE	3.2
1	E	448	VAL	3.2
1	F	142	VAL	3.2
1	B	427	GLY	3.2
1	A	102	ASP	3.2
1	A	217	ASP	3.2
1	E	117	TYR	3.2
1	E	496	TYR	3.2
1	E	34	VAL	3.2
1	C	41	LYS	3.2
1	F	243	MSE	3.2
1	E	292	ALA	3.2
1	F	129	ASP	3.2
1	D	351	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	162	LYS	3.2
1	F	256	GLN	3.2
1	C	77	VAL	3.2
1	F	226	PRO	3.2
1	E	49	LYS	3.2
1	E	59	THR	3.2
1	F	343	ARG	3.2
1	E	190	PRO	3.2
1	F	319	ALA	3.2
1	B	465	LYS	3.2
1	E	280	ASN	3.2
1	B	227	VAL	3.2
1	D	70	VAL	3.2
1	F	277	PRO	3.2
1	C	230	ALA	3.2
1	C	409	VAL	3.2
1	D	342	VAL	3.2
1	F	116	PHE	3.2
1	E	147	THR	3.2
1	B	354	LEU	3.2
1	A	358	ILE	3.2
1	F	55	ILE	3.2
1	F	91	ASN	3.2
1	F	53	PHE	3.1
1	B	332	PRO	3.1
1	B	462	LEU	3.1
1	F	219	SER	3.1
1	F	444	ILE	3.1
1	A	255	LEU	3.1
1	B	241	SER	3.1
1	B	113	ARG	3.1
1	E	76	ALA	3.1
1	B	155	ILE	3.1
1	B	377	GLY	3.1
1	C	116	PHE	3.1
1	E	480	GLN	3.1
1	A	349	THR	3.1
1	D	227	VAL	3.1
1	D	462	LEU	3.1
1	F	54	LYS	3.1
1	F	414	HIS	3.1
1	C	256	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	172	ASP	3.1
1	E	459	TYR	3.1
1	F	218	GLU	3.1
1	D	59	THR	3.1
1	F	70	VAL	3.1
1	A	103	LEU	3.1
1	D	303	SER	3.1
1	F	118	GLY	3.1
1	E	251	ASP	3.1
1	A	227	VAL	3.1
1	A	364	SER	3.1
1	B	21	VAL	3.1
1	C	413	ASP	3.1
1	D	389	SER	3.1
1	E	176	PRO	3.1
1	F	137	LEU	3.1
1	D	230	ALA	3.1
1	C	402	ILE	3.1
1	F	47	HIS	3.1
1	F	5	PHE	3.1
1	E	295	LYS	3.1
1	E	330	LEU	3.1
1	E	462	LEU	3.1
1	B	195	GLY	3.1
1	D	171	HIS	3.1
1	E	241	SER	3.0
1	B	239	LEU	3.0
1	E	482	LEU	3.0
1	B	471	ASN	3.0
1	B	101	PHE	3.0
1	B	81	THR	3.0
1	D	71	LEU	3.0
1	D	108	LEU	3.0
1	E	3	LEU	3.0
1	E	112	LEU	3.0
1	F	258	GLY	3.0
1	C	265	ALA	3.0
1	F	430	ASP	3.0
1	B	461	GLU	3.0
1	A	58	PHE	3.0
1	A	324	PHE	3.0
1	F	239	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	165	LYS	3.0
1	B	265	ALA	3.0
1	A	357	ASP	3.0
1	E	314	ILE	3.0
1	C	324	PHE	3.0
1	F	298	ARG	3.0
1	D	199	VAL	3.0
1	F	120	VAL	3.0
1	F	159	LEU	3.0
1	F	456	LEU	3.0
1	F	211	ARG	3.0
1	F	231	ILE	3.0
1	B	87	LYS	3.0
1	D	134	GLY	3.0
1	E	377	GLY	3.0
1	A	36	PRO	3.0
1	B	197	PRO	3.0
1	C	277	PRO	3.0
1	E	475	CYS	3.0
1	B	40	ALA	3.0
1	F	153	ASP	3.0
1	A	167	ILE	3.0
1	C	206	ILE	3.0
1	D	376	ILE	3.0
1	C	478	PHE	3.0
1	A	91	ASN	3.0
1	B	146	PRO	3.0
1	D	92	LEU	3.0
1	E	138	PRO	3.0
1	C	250	LYS	3.0
1	D	83	TYR	3.0
1	D	202	ASP	3.0
1	A	182	ARG	3.0
1	E	165	LYS	3.0
1	E	300	LYS	3.0
1	B	167	ILE	3.0
1	C	378	GLY	3.0
1	A	79	PHE	3.0
1	A	293	LEU	3.0
1	A	262	VAL	3.0
1	E	130	VAL	3.0
1	E	243	MSE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	474	CYS	3.0
1	C	289	ALA	3.0
1	F	121	ASP	3.0
1	C	83	TYR	3.0
1	E	104	HIS	3.0
1	B	6	ILE	2.9
1	D	144	ILE	2.9
1	A	436	PRO	2.9
1	E	197	PRO	2.9
1	D	81	THR	2.9
1	F	387	TYR	2.9
1	C	60	GLY	2.9
1	D	306	SER	2.9
1	D	348	ILE	2.9
1	C	18	ASN	2.9
1	C	79	PHE	2.9
1	E	270	LEU	2.9
1	F	108	LEU	2.9
1	D	130	VAL	2.9
1	F	413	ASP	2.9
1	D	117	TYR	2.9
1	E	55	ILE	2.9
1	E	478	PHE	2.9
1	F	301	PHE	2.9
1	F	21	VAL	2.9
1	E	271	GLY	2.9
1	B	424	SER	2.9
1	E	106	SER	2.9
1	D	42	ARG	2.9
1	D	460	LEU	2.9
1	A	207	VAL	2.9
1	C	285	VAL	2.9
1	D	381	ASP	2.9
1	D	325	LYS	2.9
1	E	139	THR	2.9
1	F	157	VAL	2.9
1	F	169	GLY	2.9
1	F	24	SER	2.9
1	C	177	LEU	2.9
1	B	347	VAL	2.9
1	F	34	VAL	2.9
1	B	230	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	466	GLY	2.9
1	E	146	PRO	2.9
1	F	176	PRO	2.9
1	A	342	VAL	2.9
1	C	471	ASN	2.9
1	A	23	PHE	2.9
1	E	167	ILE	2.9
1	F	177	LEU	2.9
1	B	258	GLY	2.9
1	C	134	GLY	2.9
1	F	312	SER	2.9
1	F	51	ASN	2.9
1	C	108	LEU	2.8
1	E	291	ILE	2.8
1	B	182	ARG	2.8
1	A	235	VAL	2.8
1	B	367	VAL	2.8
1	C	375	GLY	2.8
1	D	283	THR	2.8
1	F	468	THR	2.8
1	D	412	HIS	2.8
1	D	483	ALA	2.8
1	D	432	ARG	2.8
1	E	371	ARG	2.8
1	A	112	LEU	2.8
1	E	407	PRO	2.8
1	A	370	THR	2.8
1	B	29	ALA	2.8
1	A	251	ASP	2.8
1	C	185	LEU	2.8
1	C	258	GLY	2.8
1	E	341	ILE	2.8
1	E	282	TYR	2.8
1	E	378	GLY	2.8
1	B	189	THR	2.8
1	C	140	THR	2.8
1	D	98	THR	2.8
1	D	31	ASN	2.8
1	F	73	GLN	2.8
1	F	293	LEU	2.8
1	D	124	ILE	2.8
1	B	235	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	17	HIS	2.8
1	C	309	VAL	2.8
1	E	412	HIS	2.8
1	E	320	ASN	2.8
1	B	184	GLU	2.8
1	C	315	GLN	2.8
1	F	315	GLN	2.8
1	B	369	GLY	2.8
1	F	244	LYS	2.8
1	B	248	ILE	2.8
1	B	262	VAL	2.8
1	B	352	THR	2.8
1	B	320	ASN	2.8
1	C	237	ALA	2.8
1	D	9	GLU	2.8
1	D	216	ASN	2.8
1	F	160	ASN	2.8
1	B	107	THR	2.8
1	C	187	VAL	2.8
1	C	467	GLN	2.8
1	C	275	ASP	2.8
1	C	143	GLY	2.7
1	B	402	ILE	2.7
1	B	325	LYS	2.7
1	C	117	TYR	2.7
1	C	306	SER	2.7
1	C	325	LYS	2.7
1	D	165	LYS	2.7
1	E	244	LYS	2.7
1	F	434	LYS	2.7
1	D	273	ASN	2.7
1	A	45	ALA	2.7
1	A	326	ASP	2.7
1	C	45	ALA	2.7
1	E	476	PHE	2.7
1	C	167	ILE	2.7
1	C	335	TYR	2.7
1	A	356	ALA	2.7
1	C	430	ASP	2.7
1	A	427	GLY	2.7
1	C	208	GLY	2.7
1	F	154	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	327	LYS	2.7
1	A	82	PRO	2.7
1	C	220	ASP	2.7
1	E	451	ASP	2.7
1	F	233	ASP	2.7
1	D	2	ALA	2.7
1	F	401	LYS	2.7
1	B	173	LEU	2.7
1	C	330	LEU	2.7
1	E	137	LEU	2.7
1	E	177	LEU	2.7
1	F	391	PHE	2.7
1	C	248	ILE	2.7
1	E	348	ILE	2.7
1	F	6	ILE	2.7
1	F	140	THR	2.7
1	C	201	VAL	2.7
1	D	232	GLY	2.7
1	F	461	GLU	2.7
1	B	456	LEU	2.7
1	C	73	GLN	2.7
1	C	299	ILE	2.7
1	D	368	SER	2.7
1	E	86	ASN	2.7
1	E	479	HIS	2.7
1	F	106	SER	2.7
1	C	383	THR	2.7
1	D	158	GLU	2.7
1	E	220	ASP	2.7
1	F	225	ASP	2.7
1	F	344	ARG	2.7
1	D	290	VAL	2.7
1	E	285	VAL	2.7
1	E	397	MSE	2.7
1	F	35	VAL	2.7
1	E	265	ALA	2.7
1	C	476	PHE	2.7
1	E	82	PRO	2.7
1	E	254	PRO	2.7
1	B	288	ASP	2.7
1	B	317	ILE	2.7
1	B	358	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	444	ILE	2.7
1	E	208	GLY	2.7
1	D	323	PHE	2.7
1	B	374	ASN	2.7
1	A	291	ILE	2.7
1	F	217	ASP	2.7
1	F	333	GLN	2.7
1	B	270	LEU	2.6
1	B	450	PRO	2.6
1	D	379	SER	2.6
1	D	362	ILE	2.6
1	A	165	LYS	2.6
1	A	388	VAL	2.6
1	F	419	VAL	2.6
1	E	40	ALA	2.6
1	C	431	LEU	2.6
1	C	482	LEU	2.6
1	D	197	PRO	2.6
1	C	303	SER	2.6
1	D	192	ASP	2.6
1	E	133	ASP	2.6
1	E	219	SER	2.6
1	E	433	GLY	2.6
1	C	370	THR	2.6
1	F	349	THR	2.6
1	C	342	VAL	2.6
1	E	193	ARG	2.6
1	F	204	ALA	2.6
1	A	282	TYR	2.6
1	B	137	LEU	2.6
1	E	281	MSE	2.6
1	A	471	ASN	2.6
1	B	23	PHE	2.6
1	E	180	PRO	2.6
1	F	450	PRO	2.6
1	B	174	CYS	2.6
1	C	64	GLY	2.6
1	D	169	GLY	2.6
1	E	369	GLY	2.6
1	E	403	SER	2.6
1	F	195	GLY	2.6
1	A	231	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	147	THR	2.6
1	A	201	VAL	2.6
1	B	201	VAL	2.6
1	B	108	LEU	2.6
1	A	101	PHE	2.6
1	B	217	ASP	2.6
1	B	274	PRO	2.6
1	C	68	ASP	2.6
1	C	234	ASN	2.6
1	C	246	GLY	2.6
1	C	415	SER	2.6
1	D	56	GLY	2.6
1	D	436	PRO	2.6
1	D	479	HIS	2.6
1	D	340	GLU	2.6
1	A	475	CYS	2.6
1	F	39	ILE	2.6
1	F	125	ILE	2.6
1	F	392	THR	2.6
1	E	87	LYS	2.6
1	A	267	LEU	2.6
1	A	220	ASP	2.6
1	B	100	TYR	2.6
1	B	435	ASN	2.6
1	D	387	TYR	2.6
1	F	487	ASP	2.6
1	B	392	THR	2.6
1	B	422	ILE	2.6
1	E	358	ILE	2.6
1	C	472	LEU	2.6
1	C	494	GLU	2.6
1	D	60	GLY	2.6
1	A	219	SER	2.6
1	C	42	ARG	2.6
1	D	364	SER	2.6
1	B	362	ILE	2.6
1	C	6	ILE	2.6
1	D	314	ILE	2.6
1	C	347	VAL	2.6
1	F	347	VAL	2.6
1	B	76	ALA	2.6
1	F	43	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	466	GLY	2.6
1	D	251	ASP	2.6
1	E	25	GLY	2.6
1	E	381	ASP	2.6
1	E	463	GLY	2.6
1	E	279	PHE	2.6
1	F	198	TYR	2.6
1	C	81	THR	2.6
1	E	39	ILE	2.6
1	A	265	ALA	2.6
1	D	145	LEU	2.5
1	B	338	ASN	2.5
1	F	20	ASN	2.5
1	C	394	PRO	2.5
1	F	180	PRO	2.5
1	A	423	ILE	2.5
1	B	148	ILE	2.5
1	E	44	ILE	2.5
1	E	362	ILE	2.5
1	D	209	VAL	2.5
1	B	371	ARG	2.5
1	E	45	ALA	2.5
1	B	297	GLY	2.5
1	F	297	GLY	2.5
1	C	241	SER	2.5
1	D	312	SER	2.5
1	D	424	SER	2.5
1	D	405	PHE	2.5
1	A	465	LYS	2.5
1	E	135	LYS	2.5
1	E	158	GLU	2.5
1	F	126	GLU	2.5
1	A	136	ILE	2.5
1	A	156	ILE	2.5
1	A	362	ILE	2.5
1	A	422	ILE	2.5
1	D	189	THR	2.5
1	E	155	ILE	2.5
1	A	128	ALA	2.5
1	D	222	ALA	2.5
1	E	367	VAL	2.5
1	E	294	MSE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	64	GLY	2.5
1	A	270	LEU	2.5
1	A	218	GLU	2.5
1	C	5	PHE	2.5
1	F	442	GLU	2.5
1	A	84	GLN	2.5
1	A	124	ILE	2.5
1	A	456	LEU	2.5
1	D	172	ASP	2.5
1	C	484	LYS	2.5
1	B	324	PHE	2.5
1	A	383	THR	2.5
1	F	206	ILE	2.5
1	F	474	CYS	2.5
1	B	68	ASP	2.5
1	B	220	ASP	2.5
1	A	31	ASN	2.5
1	C	236	ALA	2.5
1	E	316	ASP	2.5
1	B	185	LEU	2.5
1	D	330	LEU	2.5
1	E	145	LEU	2.5
1	F	31	ASN	2.5
1	F	87	LYS	2.5
1	F	460	LEU	2.5
1	B	191	SER	2.5
1	F	415	SER	2.5
1	D	200	GLN	2.5
1	F	113	ARG	2.5
1	A	360	GLY	2.5
1	D	341	ILE	2.5
1	E	195	GLY	2.5
1	A	20	ASN	2.5
1	C	361	ASN	2.5
1	D	309	VAL	2.5
1	F	135	LYS	2.5
1	D	218	GLU	2.5
1	F	48	GLU	2.5
1	F	82	PRO	2.5
1	F	249	PRO	2.5
1	B	322	ASP	2.5
1	B	309	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	390	ILE	2.5
1	B	423	ILE	2.5
1	F	365	THR	2.5
1	E	262	VAL	2.5
1	E	313	VAL	2.5
1	F	342	VAL	2.5
1	A	301	PHE	2.5
1	C	58	PHE	2.5
1	A	168	MSE	2.5
1	C	373	MSE	2.5
1	A	352	THR	2.5
1	F	220	ASP	2.5
1	A	320	ASN	2.5
1	C	125	ILE	2.5
1	A	493	TRP	2.4
1	E	331	ARG	2.4
1	E	440	ALA	2.5
1	F	222	ALA	2.5
1	A	163	HIS	2.4
1	A	305	CYS	2.4
1	F	186	PRO	2.4
1	C	142	VAL	2.4
1	C	155	ILE	2.4
1	C	493	TRP	2.4
1	F	484	LYS	2.4
1	C	366	HIS	2.4
1	E	332	PRO	2.4
1	E	366	HIS	2.4
1	B	405	PHE	2.4
1	A	447	CYS	2.4
1	E	56	GLY	2.4
1	F	287	GLN	2.4
1	D	27	THR	2.4
1	A	144	ILE	2.4
1	D	89	LEU	2.4
1	D	402	ILE	2.4
1	D	423	ILE	2.4
1	B	271	GLY	2.4
1	C	463	GLY	2.4
1	D	213	SER	2.4
1	E	187	VAL	2.4
1	E	406	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	191	SER	2.4
1	F	431	LEU	2.4
1	B	83	TYR	2.4
1	E	175	GLU	2.4
1	F	158	GLU	2.4
1	F	438	GLU	2.4
1	C	179	PRO	2.4
1	E	171	HIS	2.4
1	A	279	PHE	2.4
1	A	484	LYS	2.4
1	F	78	LYS	2.4
1	F	196	LYS	2.4
1	A	467	GLN	2.4
1	B	283	THR	2.4
1	E	284	GLU	2.4
1	B	15	VAL	2.4
1	D	406	VAL	2.4
1	F	109	ALA	2.4
1	D	100	TYR	2.4
1	A	193	ARG	2.4
1	E	417	HIS	2.4
1	E	449	HIS	2.4
1	A	233	ASP	2.4
1	D	86	ASN	2.4
1	E	94	ASN	2.4
1	E	124	ILE	2.4
1	E	390	ILE	2.4
1	E	431	LEU	2.4
1	F	310	SER	2.4
1	A	204	ALA	2.4
1	B	408	MSE	2.4
1	D	331	ARG	2.4
1	D	360	GLY	2.4
1	A	164	PRO	2.4
1	A	274	PRO	2.4
1	E	315	GLN	2.4
1	C	301	PHE	2.4
1	D	161	ASP	2.4
1	E	58	PHE	2.4
1	E	234	ASN	2.4
1	A	283	THR	2.4
1	E	283	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	306	SER	2.4
1	B	240	VAL	2.4
1	C	276	ILE	2.4
1	D	157	VAL	2.4
1	D	347	VAL	2.4
1	E	429	ALA	2.4
1	F	448	VAL	2.4
1	B	117	TYR	2.4
1	B	412	HIS	2.4
1	B	426	TRP	2.4
1	F	164	PRO	2.4
1	B	284	GLU	2.4
1	E	374	ASN	2.4
1	F	205	LYS	2.4
1	A	404	SER	2.4
1	D	62	SER	2.4
1	B	89	LEU	2.4
1	B	460	LEU	2.4
1	C	59	THR	2.4
1	C	393	THR	2.4
1	E	384	ARG	2.4
1	D	358	ILE	2.3
1	C	82	PRO	2.3
1	C	171	HIS	2.3
1	D	414	HIS	2.3
1	E	391	PHE	2.3
1	A	95	ASN	2.3
1	E	338	ASN	2.3
1	C	139	THR	2.3
1	B	50	GLY	2.3
1	B	440	ALA	2.3
1	E	443	ILE	2.3
1	F	236	ALA	2.3
1	E	484	LYS	2.3
1	C	272	ASP	2.3
1	E	288	ASP	2.3
1	F	272	ASP	2.3
1	F	469	PRO	2.3
1	C	273	ASN	2.3
1	E	4	ARG	2.3
1	F	352	THR	2.3
1	B	232	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	236	ALA	2.3
1	B	291	ILE	2.3
1	C	72	ALA	2.3
1	C	207	VAL	2.3
1	D	45	ALA	2.3
1	E	396	VAL	2.3
1	A	180	PRO	2.3
1	A	450	PRO	2.3
1	D	430	ASP	2.3
1	D	23	PHE	2.3
1	D	481	GLU	2.3
1	E	250	LYS	2.3
1	F	364	SER	2.3
1	F	115	GLY	2.3
1	F	141	GLY	2.3
1	F	354	LEU	2.3
1	B	285	VAL	2.3
1	E	299	ILE	2.3
1	C	371	ARG	2.3
1	E	32	PRO	2.3
1	C	300	LYS	2.3
1	F	355	GLU	2.3
1	B	145	LEU	2.3
1	C	71	LEU	2.3
1	C	307	LEU	2.3
1	A	74	ALA	2.3
1	B	259	VAL	2.3
1	C	240	VAL	2.3
1	C	353	ALA	2.3
1	E	174	CYS	2.3
1	C	217	ASP	2.3
1	D	104	HIS	2.3
1	D	343	ARG	2.3
1	E	357	ASP	2.3
1	F	451	ASP	2.3
1	B	205	LYS	2.3
1	E	205	LYS	2.3
1	E	490	ASN	2.3
1	F	470	GLN	2.3
1	A	100	TYR	2.3
1	E	494	GLU	2.3
1	C	485	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	368	SER	2.3
1	B	482	LEU	2.3
1	B	152	ALA	2.3
1	B	487	ASP	2.3
1	C	128	ALA	2.3
1	E	122	VAL	2.3
1	F	102	ASP	2.3
1	E	441	HIS	2.3
1	F	174	CYS	2.3
1	C	126	GLU	2.3
1	D	36	PRO	2.3
1	E	23	PHE	2.3
1	B	114	TYR	2.3
1	E	493	TRP	2.3
1	D	415	SER	2.3
1	D	173	LEU	2.3
1	D	298	ARG	2.3
1	D	311	ARG	2.3
1	D	484	LYS	2.3
1	D	155	ILE	2.3
1	E	126	GLU	2.3
1	C	197	PRO	2.3
1	C	450	PRO	2.3
1	D	5	PHE	2.3
1	E	97	SER	2.3
1	E	325	LYS	2.3
1	F	241	SER	2.3
1	E	473	ASP	2.2
1	A	266	VAL	2.2
1	B	120	VAL	2.2
1	F	406	VAL	2.2
1	B	444	ILE	2.2
1	B	213	SER	2.2
1	D	475	CYS	2.2
1	F	463	GLY	2.2
1	F	486	GLY	2.2
1	C	282	TYR	2.2
1	D	282	TYR	2.2
1	C	255	LEU	2.2
1	D	105	LEU	2.2
1	E	71	LEU	2.2
1	F	145	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	37	ALA	2.2
1	B	299	ILE	2.2
1	C	55	ILE	2.2
1	F	250	LYS	2.2
1	E	346	GLY	2.2
1	E	439	ARG	2.2
1	F	42	ARG	2.2
1	C	97	SER	2.2
1	A	149	CYS	2.2
1	F	425	GLU	2.2
1	B	307	LEU	2.2
1	C	188	TYR	2.2
1	E	387	TYR	2.2
1	F	399	ASP	2.2
1	A	35	VAL	2.2
1	A	38	ALA	2.2
1	B	142	VAL	2.2
1	B	406	VAL	2.2
1	B	428	VAL	2.2
1	C	46	ALA	2.2
1	F	302	ALA	2.2
1	C	124	ILE	2.2
1	C	341	ILE	2.2
1	F	384	ARG	2.2
1	D	85	SER	2.2
1	A	426	TRP	2.2
1	B	229	GLN	2.2
1	A	445	ASP	2.2
1	B	177	LEU	2.2
1	D	54	LYS	2.2
1	F	100	TYR	2.2
1	E	7	THR	2.2
1	A	61	ALA	2.2
1	A	210	VAL	2.2
1	D	123	ALA	2.2
1	F	171	HIS	2.2
1	A	155	ILE	2.2
1	C	158	GLU	2.2
1	E	166	GLU	2.2
1	F	481	GLU	2.2
1	C	221	PHE	2.2
1	C	382	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	170	MSE	2.2
1	A	345	LEU	2.2
1	E	293	LEU	2.2
1	A	27	THR	2.2
1	A	140	THR	2.2
1	A	419	VAL	2.2
1	B	61	ALA	2.2
1	B	216	ASN	2.2
1	C	464	VAL	2.2
1	D	265	ALA	2.2
1	E	109	ALA	2.2
1	B	190	PRO	2.2
1	B	206	ILE	2.2
1	C	443	ILE	2.2
1	E	96	GLY	2.2
1	E	404	SER	2.2
1	A	133	ASP	2.2
1	A	397	MSE	2.2
1	A	392	THR	2.2
1	C	311	ARG	2.2
1	D	459	TYR	2.2
1	E	452	TYR	2.2
1	A	157	VAL	2.2
1	B	109	ALA	2.2
1	E	355	GLU	2.2
1	E	416	GLU	2.2
1	F	9	GLU	2.2
1	A	148	ILE	2.2
1	D	250	LYS	2.2
1	E	421	VAL	2.2
1	A	53	PHE	2.2
1	A	241	SER	2.2
1	A	303	SER	2.2
1	A	403	SER	2.2
1	E	211	ARG	2.2
1	A	94	ASN	2.2
1	A	196	LYS	2.2
1	A	409	VAL	2.2
1	A	486	GLY	2.2
1	B	128	ALA	2.2
1	C	65	ALA	2.2
1	C	302	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	240	VAL	2.2
1	E	419	VAL	2.2
1	A	350	ILE	2.2
1	F	423	ILE	2.2
1	C	364	SER	2.2
1	E	191	SER	2.2
1	A	81	THR	2.1
1	A	468	THR	2.1
1	B	493	TRP	2.1
1	A	114	TYR	2.1
1	B	353	ALA	2.1
1	C	406	VAL	2.1
1	E	290	VAL	2.1
1	D	394	PRO	2.1
1	F	436	PRO	2.1
1	A	150	ARG	2.1
1	A	391	PHE	2.1
1	C	359	PHE	2.1
1	D	301	PHE	2.1
1	B	135	LYS	2.1
1	C	192	ASP	2.1
1	E	267	LEU	2.1
1	F	307	LEU	2.1
1	D	160	ASN	2.1
1	D	320	ASN	2.1
1	D	46	ALA	2.1
1	C	130	VAL	2.1
1	E	207	VAL	2.1
1	A	49	LYS	2.1
1	B	85	SER	2.1
1	E	113	ARG	2.1
1	E	298	ARG	2.1
1	A	68	ASP	2.1
1	C	102	ASP	2.1
1	C	399	ASP	2.1
1	D	382	PHE	2.1
1	B	431	LEU	2.1
1	C	195	GLY	2.1
1	D	374	ASN	2.1
1	C	468	THR	2.1
1	D	131	THR	2.1
1	D	366	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	22	GLY	2.1
1	F	98	THR	2.1
1	E	152	ALA	2.1
1	B	48	GLU	2.1
1	C	199	VAL	2.1
1	D	448	VAL	2.1
1	F	396	VAL	2.1
1	D	238	PHE	2.1
1	E	382	PHE	2.1
1	C	345	LEU	2.1
1	D	482	LEU	2.1
1	E	264	ASN	2.1
1	A	366	HIS	2.1
1	B	98	THR	2.1
1	E	140	THR	2.1
1	F	27	THR	2.1
1	C	152	ALA	2.1
1	A	77	VAL	2.1
1	D	35	VAL	2.1
1	E	215	PRO	2.1
1	E	342	VAL	2.1
1	A	424	SER	2.1
1	F	156	ILE	2.1
1	B	105	LEU	2.1
1	F	455	LEU	2.1
1	E	80	ARG	2.1
1	F	432	ARG	2.1
1	F	492	ARG	2.1
1	F	139	THR	2.1
1	F	393	THR	2.1
1	A	269	ALA	2.1
1	B	263	ALA	2.1
1	F	265	ALA	2.1
1	B	149	CYS	2.1
1	B	207	VAL	2.1
1	D	203	PRO	2.1
1	E	226	PRO	2.1
1	F	339	PRO	2.1
1	A	348	ILE	2.1
1	B	133	ASP	2.1
1	B	144	ILE	2.1
1	D	125	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	33	LYS	2.1
1	B	5	PHE	2.1
1	B	476	PHE	2.1
1	C	446	LYS	2.1
1	A	377	GLY	2.1
1	B	86	ASN	2.1
1	B	466	GLY	2.1
1	D	48	GLU	2.1
1	F	371	ARG	2.1
1	D	17	HIS	2.1
1	D	236	ALA	2.1
1	E	356	ALA	2.1
1	B	266	VAL	2.1
1	B	290	VAL	2.1
1	D	396	VAL	2.1
1	A	496	TYR	2.1
1	D	75	ASP	2.1
1	D	198	TYR	2.1
1	F	495	ASP	2.1
1	B	53	PHE	2.1
1	D	438	GLU	2.1
1	F	242	GLU	2.1
1	B	280	ASN	2.1
1	F	273	ASN	2.1
1	B	17	HIS	2.1
1	C	414	HIS	2.1
1	A	306	SER	2.1
1	E	74	ALA	2.1
1	F	12	ALA	2.1
1	E	430	ASP	2.1
1	B	14	PHE	2.1
1	B	496	TYR	2.1
1	C	154	ARG	2.1
1	D	188	TYR	2.1
1	E	359	PHE	2.1
1	A	361	ASN	2.1
1	A	431	LEU	2.1
1	B	18	ASN	2.1
1	B	293	LEU	2.1
1	A	11	ALA	2.0
1	A	85	SER	2.0
1	A	240	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	199	VAL	2.0
1	E	100	TYR	2.0
1	E	238	PHE	2.0
1	F	358	ILE	2.0
1	A	169	GLY	2.0
1	C	56	GLY	2.0
1	D	195	GLY	2.0
1	B	261	ASN	2.0
1	E	103	LEU	2.0
1	F	337	ASN	2.0
1	E	110	GLN	2.0
1	F	84	GLN	2.0
1	A	146	PRO	2.0
1	B	178	ASP	2.0
1	E	13	GLU	2.0
1	A	317	ILE	2.0
1	B	25	GLY	2.0
1	C	291	ILE	2.0
1	B	282	TYR	2.0
1	F	279	PHE	2.0
1	B	351	ASN	2.0
1	B	475	CYS	2.0
1	D	494	GLU	2.0
1	E	170	MSE	2.0
1	E	468	THR	2.0
1	F	488	MSE	2.0
1	A	225	ASP	2.0
1	B	343	ARG	2.0
1	F	111	ASP	2.0
1	A	6	ILE	2.0
1	A	286	ILE	2.0
1	A	390	ILE	2.0
1	B	79	PHE	2.0
1	C	328	ILE	2.0
1	E	252	PHE	2.0
1	E	239	LEU	2.0
1	E	489	ARG	2.0
1	B	153	ASP	2.0
1	B	172	ASP	2.0
1	C	161	ASP	2.0
1	D	106	SER	2.0
1	E	424	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	263	ALA	2.0
1	E	339	PRO	2.0
1	F	305	CYS	2.0
1	C	122	VAL	2.0
1	E	70	VAL	2.0
1	F	210	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	E	507	1/1	0.07	-3.45	15,15,15,15	0
2	ZN	D	507	1/1	0.11	-3.52	17,17,17,17	0
2	ZN	B	507	1/1	0.08	-4.26	20,20,20,20	0
2	ZN	C	507	1/1	0.10	-4.35	18,18,18,18	0
2	ZN	A	507	1/1	0.10	-5.23	16,16,16,16	0
2	ZN	E	508	1/1	0.10	-5.44	25,25,25,25	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.