



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:43 AM GMT

PDB ID : 2NVV
Title : Crystal Structure of the Putative Acetyl-CoA hydrolase/transferase PG1013 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

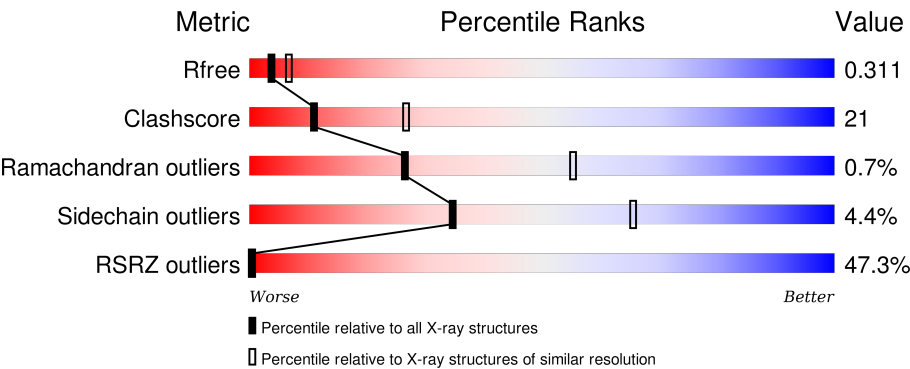
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 ≥ 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	506	<div><div>33%</div><div><div></div><div>65%</div><div>30%</div><div>..</div></div></div>
1	B	506	<div><div>40%</div><div><div></div><div>64%</div><div>31%</div><div>..</div></div></div>
1	C	506	<div><div>34%</div><div><div></div><div>65%</div><div>30%</div><div>..</div></div></div>
1	D	506	<div><div>39%</div><div><div></div><div>65%</div><div>30%</div><div>..</div></div></div>
1	E	506	<div><div>63%</div><div><div></div><div>61%</div><div>34%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	506	<div><div><div></div><div></div><div></div></div><div>62%61%34%••</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23178 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 Acetyl-CoA hydrolase/transferase family 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

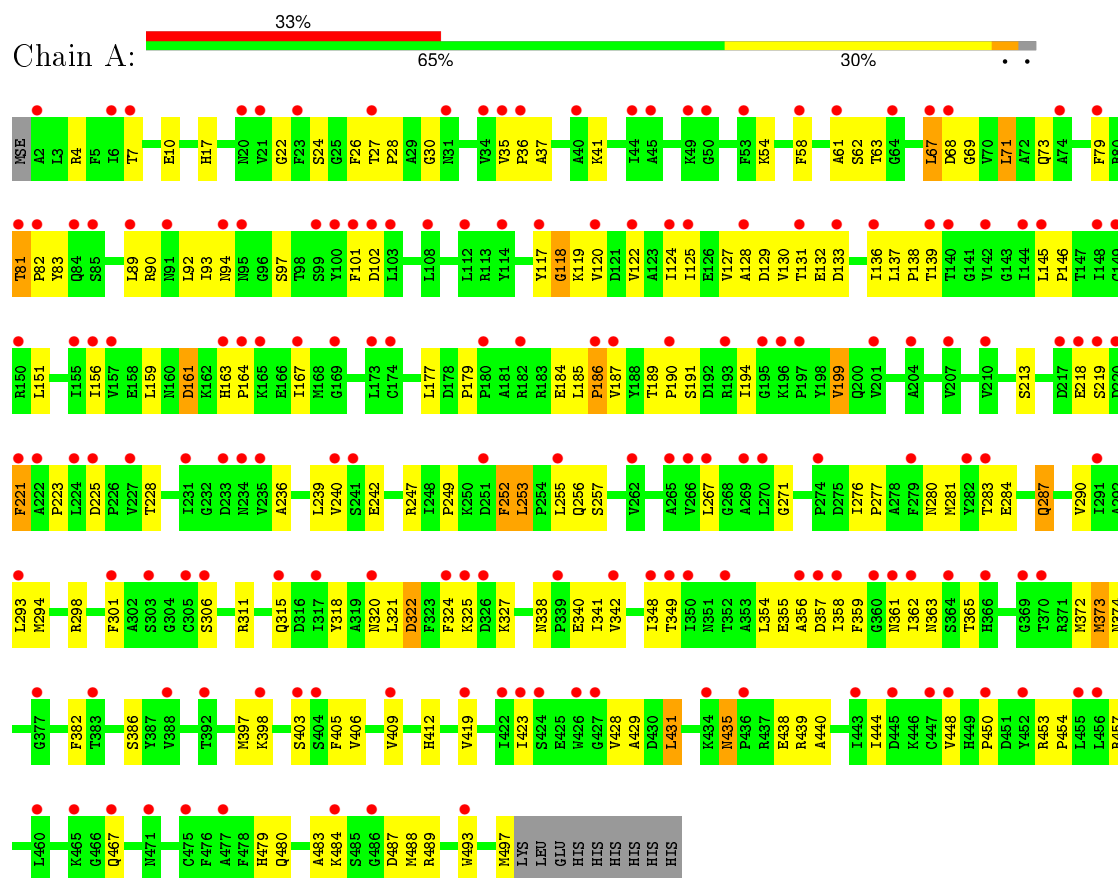
- Molecule 3 is water.

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

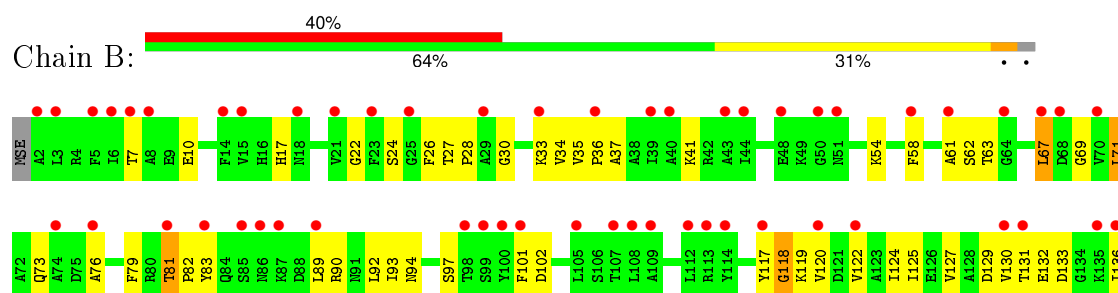
3 Residue-property plots

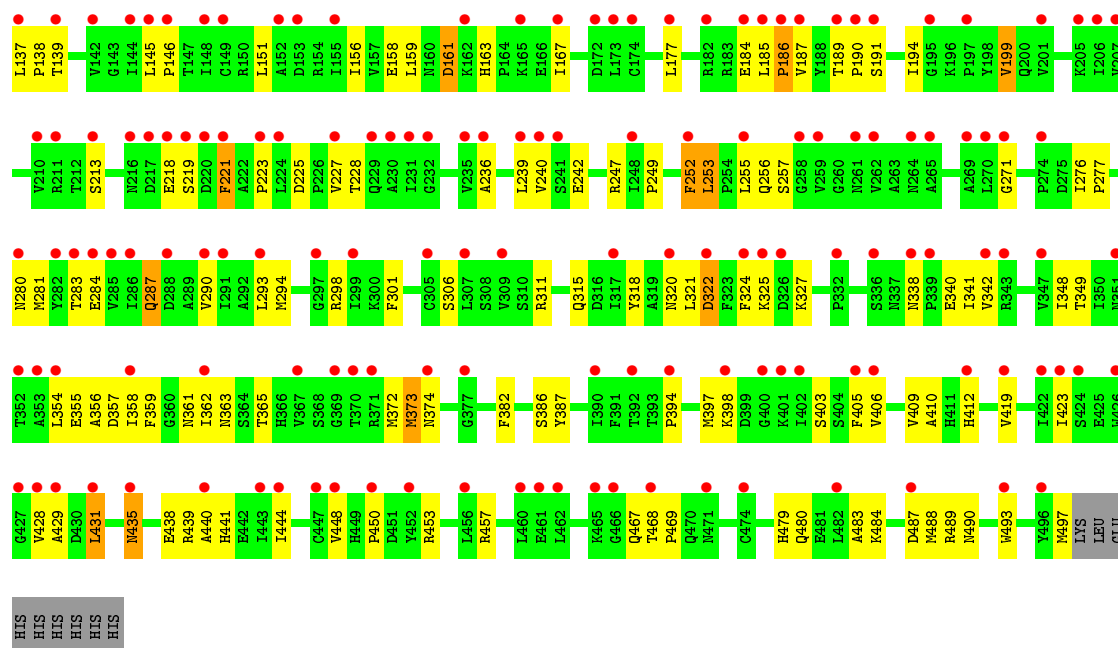
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

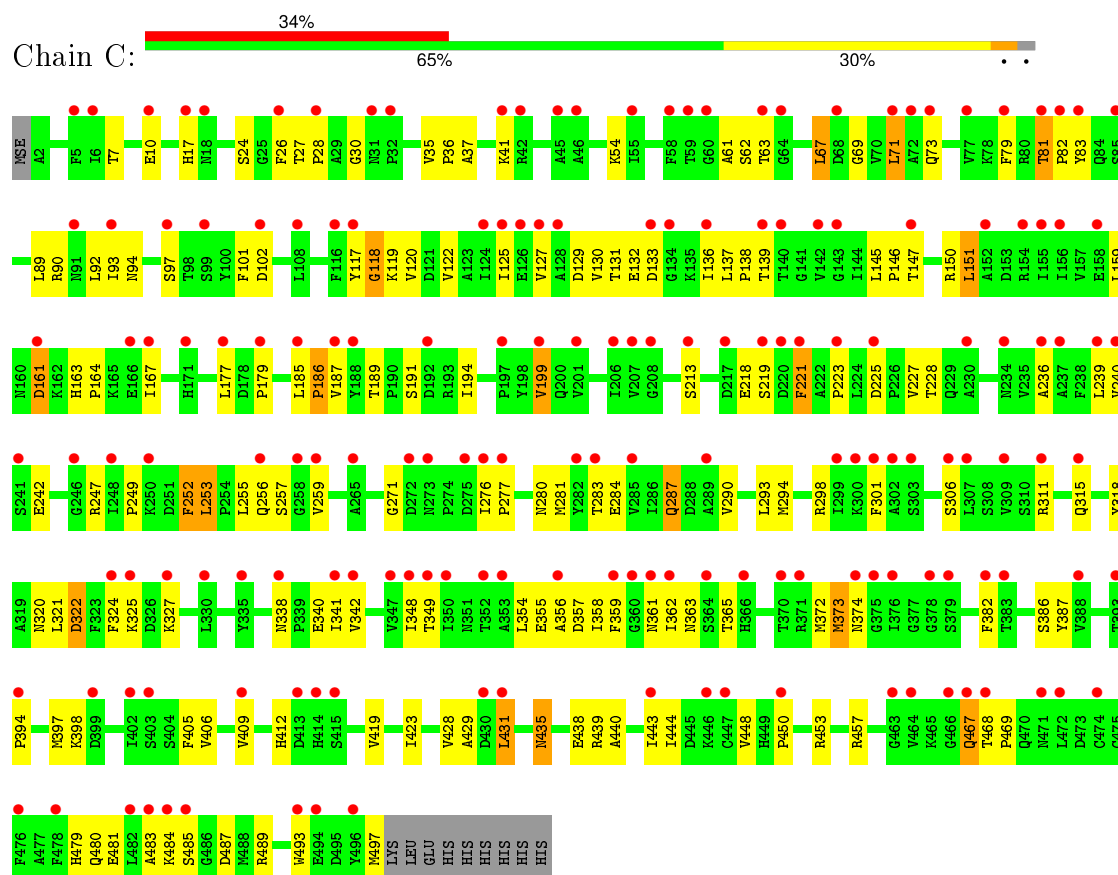


- Molecule 1: Acetyl-CoA hydrolase/transferase family protein

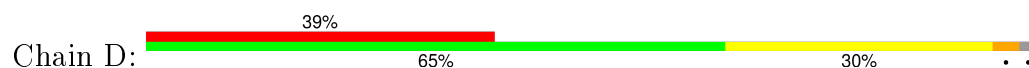


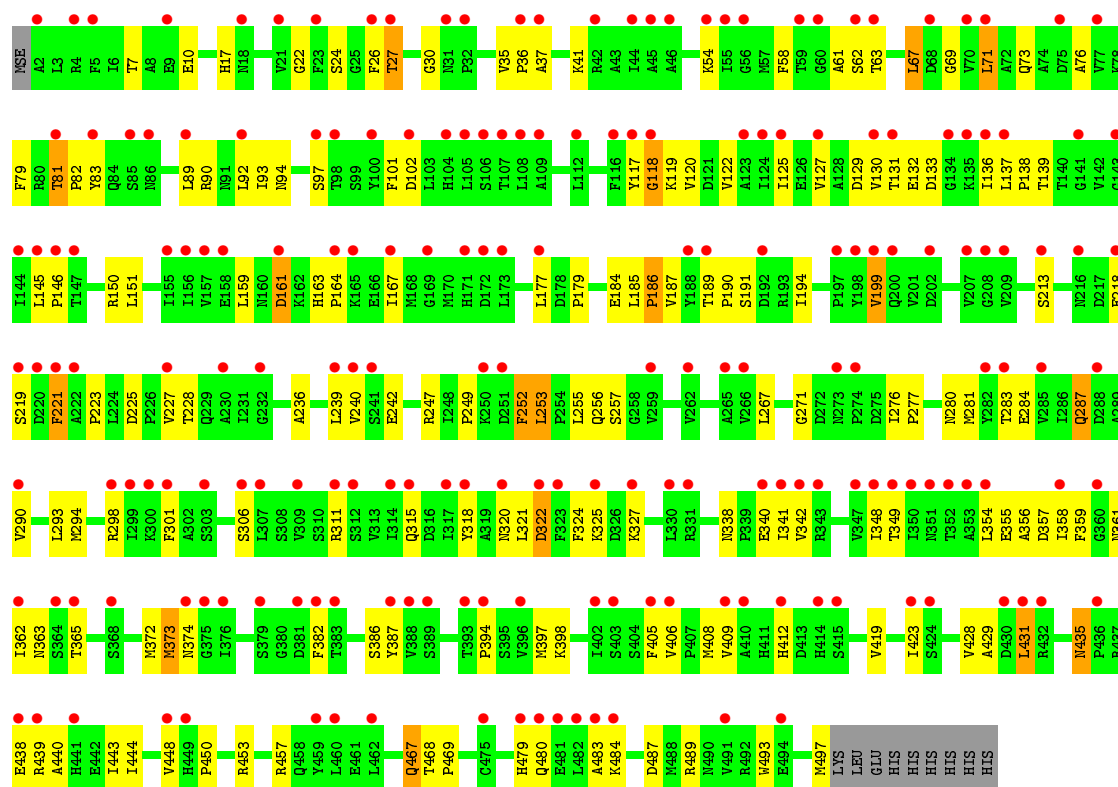


- Molecule 1: Acetyl-CoA hydrolase/transferase family protein

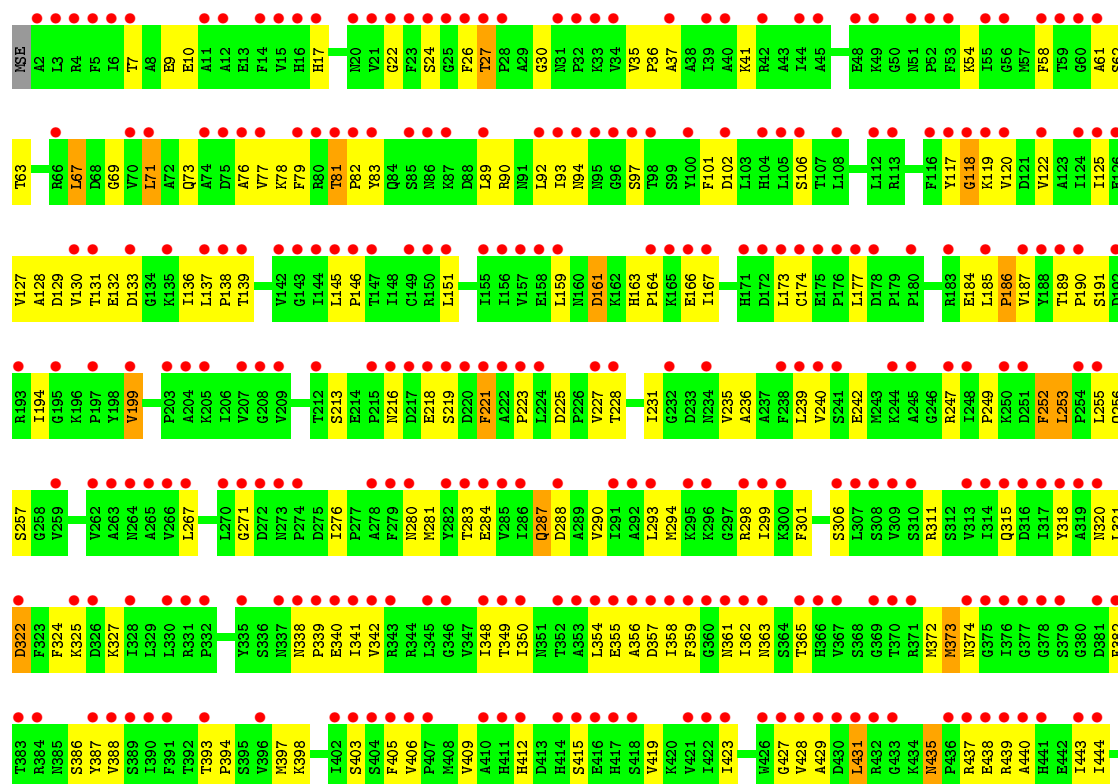


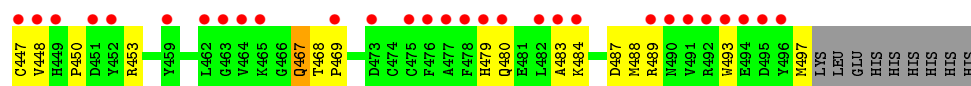
- Molecule 1: Acetyl-CoA hydrolase/transferase family protein



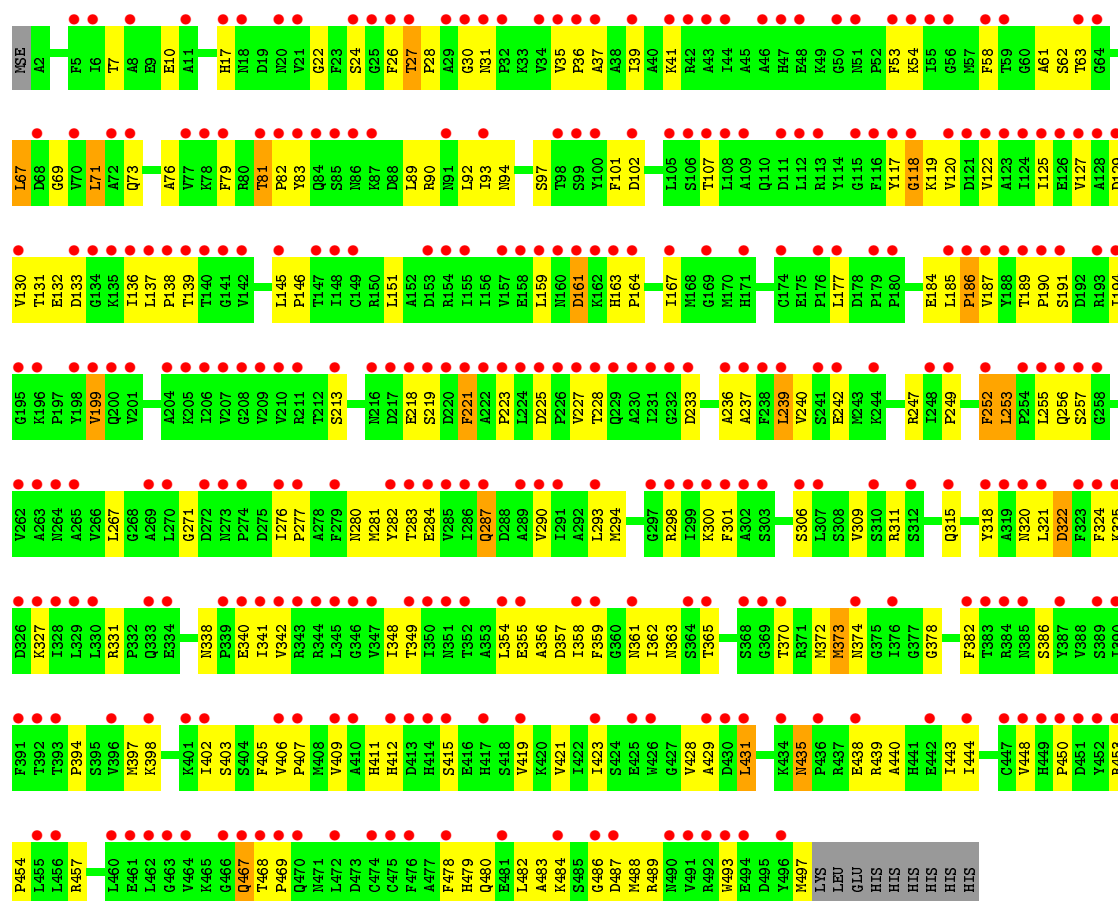


• Molecule 1: Acetyl-CoA hydrolase/transferase family protein





● Molecule 1: Acetyl-CoA hydrolase/transferase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	5.63 (at 2.39Å)	Xtriage
Refinement program	XTALVIEW, CNS 1.1	Depositor
R, R_{free}	0.287 , 0.290 0.310 , 0.311	Depositor DCC
R_{free} test set	4413 reflections (10.94%)	DCC
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , -5.5	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 ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 21.

All (957) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:THR:O	1:C:373:MSE:HB2	1.78	0.84
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	30	59
1	B	494/506 (98%)	462 (94%)	29 (6%)	3 (1%)	30	59
1	C	494/506 (98%)	460 (93%)	31 (6%)	3 (1%)	30	59
1	D	494/506 (98%)	461 (93%)	29 (6%)	4 (1%)	24	51
1	E	494/506 (98%)	461 (93%)	29 (6%)	4 (1%)	24	51
1	F	494/506 (98%)	460 (93%)	30 (6%)	4 (1%)	24	51
All	All	2964/3036 (98%)	2762 (93%)	181 (6%)	21 (1%)	26	55

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
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%)	35	66
1	B	416/413 (101%)	398 (96%)	18 (4%)	35	66
1	C	416/413 (101%)	397 (95%)	19 (5%)	33	64
1	D	416/413 (101%)	397 (95%)	19 (5%)	33	64
1	E	416/413 (101%)	398 (96%)	18 (4%)	35	66
1	F	416/413 (101%)	398 (96%)	18 (4%)	35	66
All	All	2496/2478 (101%)	2386 (96%)	110 (4%)	35	65

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	484/506 (95%)	1.80	168 (34%) 0 0	6, 7, 18, 30	0
1	B	484/506 (95%)	1.87	200 (41%) 0 0	6, 7, 18, 30	0
1	C	484/506 (95%)	1.80	174 (35%) 0 0	6, 7, 18, 30	0
1	D	484/506 (95%)	1.96	199 (41%) 0 0	6, 7, 18, 30	0
1	E	484/506 (95%)	2.63	319 (65%) 0 0	6, 7, 18, 30	0
1	F	484/506 (95%)	2.67	313 (64%) 0 0	6, 7, 18, 30	0
All	All	2904/3036 (95%)	2.12	1373 (47%) 0 0	6, 7, 18, 30	0

All (1373) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	427	GLY	8.5
1	F	134	GLY	7.6
1	F	232	GLY	7.3
1	C	85	SER	6.9
1	F	227	VAL	6.9
1	F	299	ILE	6.9
1	E	393	THR	6.6
1	E	405	PHE	6.6
1	E	365	THR	6.6
1	E	483	ALA	6.4
1	F	127	VAL	6.4
1	F	99	SER	6.4
1	F	290	VAL	6.4
1	F	149	CYS	6.3
1	E	345	LEU	6.3
1	E	383	THR	6.3
1	E	60	GLY	6.2
1	E	326	ASP	6.1
1	D	207	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
1	E	318	TYR	6.0
1	F	199	VAL	6.0
1	A	222	ALA	6.0
1	F	449	HIS	5.9
1	F	407	PRO	5.9
1	E	116	PHE	5.9
1	F	208	GLY	5.9
1	F	58	PHE	5.9
1	F	136	ILE	5.8
1	F	229	GLN	5.8
1	E	222	ALA	5.7
1	E	157	VAL	5.6
1	F	478	PHE	5.6
1	D	55	ILE	5.6
1	E	447	CYS	5.6
1	D	220	ASP	5.5
1	F	138	PRO	5.5
1	E	125	ILE	5.5
1	E	33	LYS	5.5
1	E	85	SER	5.4
1	B	122	VAL	5.4
1	C	219	SER	5.4
1	A	221	PHE	5.4
1	F	130	VAL	5.4
1	E	352	THR	5.4
1	F	270	LEU	5.4
1	F	376	ILE	5.4
1	F	328	ILE	5.4
1	F	190	PRO	5.3
1	D	410	ALA	5.3
1	F	350	ILE	5.3
1	E	203	PRO	5.3
1	F	201	VAL	5.2
1	E	217	ASP	5.2
1	F	318	TYR	5.2
1	E	477	ALA	5.2
1	F	467	GLN	5.2
1	E	370	THR	5.2
1	D	116	PHE	5.2
1	D	63	THR	5.2
1	E	363	ASN	5.2
1	A	125	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	F	382	PHE	5.1
1	D	221	PHE	5.1
1	F	494	GLU	5.1
1	D	118	GLY	5.1
1	F	462	LEU	5.1
1	F	223	PRO	5.1
1	D	307	LEU	5.1
1	F	221	PHE	5.1
1	E	89	LEU	5.1
1	E	223	PRO	5.1
1	F	496	TYR	5.0
1	D	354	LEU	5.0
1	F	447	CYS	5.0
1	F	361	ASN	5.0
1	F	123	ALA	5.0
1	F	11	ALA	5.0
1	C	350	ILE	4.9
1	F	248	ILE	4.9
1	D	352	THR	4.9
1	F	289	ALA	4.9
1	A	398	LYS	4.9
1	F	291	ILE	4.9
1	E	376	ILE	4.9
1	E	432	ARG	4.9
1	D	241	SER	4.9
1	D	137	LEU	4.9
1	D	315	GLN	4.9
1	F	274	PRO	4.9
1	F	359	PHE	4.9
1	F	286	ILE	4.9
1	F	493	TRP	4.8
1	F	255	LEU	4.8
1	E	221	PHE	4.8
1	C	376	ILE	4.8
1	E	410	ALA	4.8
1	E	322	ASP	4.8
1	F	374	ASN	4.8
1	E	52	PRO	4.8
1	F	282	TYR	4.7
1	B	2	ALA	4.7
1	F	72	ALA	4.7
1	F	230	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	119	LYS	4.7
1	F	409	VAL	4.7
1	F	383	THR	4.7
1	E	353	ALA	4.7
1	E	259	VAL	4.7
1	F	124	ILE	4.7
1	C	496	TYR	4.6
1	B	255	LEU	4.6
1	F	257	SER	4.6
1	F	148	ILE	4.6
1	F	472	LEU	4.6
1	F	263	ALA	4.6
1	E	81	THR	4.6
1	F	276	ILE	4.6
1	A	21	VAL	4.6
1	E	159	LEU	4.6
1	E	388	VAL	4.6
1	E	428	VAL	4.6
1	F	185	LEU	4.5
1	F	68	ASP	4.5
1	D	285	VAL	4.5
1	E	209	VAL	4.5
1	B	231	ILE	4.5
1	E	328	ILE	4.5
1	E	307	LEU	4.5
1	B	400	GLY	4.5
1	E	77	VAL	4.5
1	B	112	LEU	4.5
1	F	85	SER	4.5
1	B	221	PHE	4.5
1	C	374	ASN	4.5
1	E	464	VAL	4.5
1	F	117	TYR	4.5
1	B	99	SER	4.5
1	F	209	VAL	4.5
1	B	43	ALA	4.4
1	E	204	ALA	4.4
1	F	193	ARG	4.4
1	F	325	LYS	4.4
1	A	34	VAL	4.4
1	F	491	VAL	4.4
1	B	370	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	50	GLY	4.4
1	D	449	HIS	4.4
1	F	426	TRP	4.4
1	E	224	LEU	4.4
1	A	40	ALA	4.4
1	E	2	ALA	4.4
1	A	186	PRO	4.4
1	F	323	PHE	4.4
1	D	318	TYR	4.4
1	E	102	ASP	4.3
1	F	188	TYR	4.3
1	F	238	PHE	4.3
1	C	63	THR	4.3
1	F	8	ALA	4.3
1	F	207	VAL	4.3
1	A	477	ALA	4.3
1	E	354	LEU	4.3
1	E	21	VAL	4.3
1	E	185	LEU	4.3
1	E	309	VAL	4.3
1	F	326	ASP	4.2
1	E	14	PHE	4.2
1	A	117	TYR	4.2
1	B	452	TYR	4.2
1	E	422	ILE	4.2
1	D	32	PRO	4.2
1	F	59	THR	4.2
1	E	492	ARG	4.2
1	D	112	LEU	4.2
1	D	147	THR	4.2
1	F	269	ALA	4.2
1	D	136	ILE	4.2
1	D	327	LYS	4.2
1	B	7	THR	4.2
1	C	93	ILE	4.2
1	D	167	ILE	4.2
1	E	151	LEU	4.2
1	E	12	ALA	4.1
1	F	327	LYS	4.1
1	E	360	GLY	4.1
1	F	194	ILE	4.1
1	E	469	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	365	THR	4.1
1	A	2	ALA	4.1
1	E	42	ARG	4.1
1	F	264	ASN	4.1
1	E	178	ASP	4.1
1	A	173	LEU	4.1
1	F	112	LEU	4.1
1	C	352	THR	4.1
1	E	349	THR	4.1
1	C	32	PRO	4.1
1	F	228	THR	4.1
1	E	319	ALA	4.1
1	E	337	ASN	4.1
1	B	326	ASP	4.0
1	D	21	VAL	4.0
1	F	77	VAL	4.0
1	F	351	ASN	4.0
1	F	330	LEU	4.0
1	E	24	SER	4.0
1	E	418	SER	4.0
1	F	63	THR	4.0
1	C	99	SER	4.0
1	B	8	ALA	4.0
1	F	329	LEU	4.0
1	E	296	LYS	4.0
1	D	491	VAL	4.0
1	E	240	VAL	4.0
1	D	393	THR	4.0
1	E	98	THR	4.0
1	E	379	SER	4.0
1	E	415	SER	4.0
1	F	410	ALA	4.0
1	A	339	PRO	4.0
1	D	156	ILE	4.0
1	E	75	ASP	4.0
1	E	118	GLY	3.9
1	E	144	ILE	3.9
1	E	188	TYR	3.9
1	A	7	THR	3.9
1	D	388	VAL	3.9
1	E	278	ALA	3.9
1	B	58	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	99	SER	3.9
1	D	350	ILE	3.9
1	F	475	CYS	3.9
1	E	340	GLU	3.9
1	A	369	GLY	3.9
1	F	30	GLY	3.9
1	F	300	LYS	3.9
1	E	389	SER	3.9
1	F	284	GLU	3.9
1	E	173	LEU	3.9
1	D	322	ASP	3.9
1	F	161	ASP	3.9
1	D	37	ALA	3.9
1	D	18	ASN	3.9
1	E	423	ILE	3.9
1	B	3	LEU	3.9
1	C	349	THR	3.9
1	F	122	VAL	3.9
1	E	218	GLU	3.9
1	E	228	THR	3.9
1	A	64	GLY	3.9
1	B	448	VAL	3.8
1	D	146	PRO	3.8
1	F	402	ILE	3.8
1	D	349	THR	3.8
1	E	411	HIS	3.8
1	F	107	THR	3.8
1	B	286	ILE	3.8
1	E	108	LEU	3.8
1	B	342	VAL	3.8
1	F	187	VAL	3.8
1	E	286	ILE	3.8
1	E	17	HIS	3.8
1	E	66	ARG	3.8
1	E	143	GLY	3.8
1	A	120	VAL	3.8
1	E	26	PHE	3.8
1	E	61	ALA	3.8
1	A	455	LEU	3.8
1	E	93	ILE	3.8
1	F	44	ILE	3.8
1	A	67	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	350	ILE	3.8
1	E	27	THR	3.8
1	B	64	GLY	3.7
1	E	6	ILE	3.7
1	F	41	LYS	3.7
1	F	213	SER	3.7
1	E	212	THR	3.7
1	F	128	ALA	3.7
1	D	431	LEU	3.7
1	E	51	ASN	3.7
1	E	361	ASN	3.7
1	F	147	THR	3.7
1	C	28	PRO	3.7
1	E	142	VAL	3.7
1	E	95	ASN	3.7
1	F	370	THR	3.7
1	B	339	PRO	3.7
1	D	26	PHE	3.7
1	C	403	SER	3.7
1	E	156	ILE	3.7
1	F	412	HIS	3.7
1	A	131	THR	3.7
1	A	122	VAL	3.7
1	E	79	PHE	3.7
1	F	36	PRO	3.7
1	A	187	VAL	3.7
1	E	199	VAL	3.7
1	A	452	TYR	3.7
1	E	255	LEU	3.7
1	F	155	ILE	3.7
1	D	383	THR	3.7
1	A	197	PRO	3.7
1	C	360	GLY	3.7
1	C	136	ILE	3.7
1	E	92	LEU	3.6
1	A	443	ILE	3.6
1	C	133	ASP	3.6
1	F	252	PHE	3.6
1	F	46	ALA	3.6
1	D	77	VAL	3.6
1	F	83	TYR	3.6
1	F	167	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	53	PHE	3.6
1	F	283	THR	3.6
1	E	49	LYS	3.6
1	B	36	PRO	3.6
1	D	317	ILE	3.6
1	E	31	ASN	3.6
1	E	216	ASN	3.6
1	D	102	ASP	3.6
1	A	195	GLY	3.6
1	E	375	GLY	3.6
1	B	218	GLU	3.6
1	E	335	TYR	3.6
1	F	389	SER	3.6
1	D	300	LYS	3.6
1	E	15	VAL	3.6
1	F	464	VAL	3.6
1	C	239	LEU	3.5
1	E	189	THR	3.5
1	F	26	PHE	3.5
1	F	179	PRO	3.5
1	F	200	GLN	3.5
1	B	305	CYS	3.5
1	D	239	LEU	3.5
1	F	321	LEU	3.5
1	C	223	PRO	3.5
1	E	16	HIS	3.5
1	E	438	GLU	3.5
1	F	224	LEU	3.5
1	E	414	HIS	3.5
1	B	186	PRO	3.5
1	D	164	PRO	3.5
1	E	28	PRO	3.5
1	E	164	PRO	3.5
1	E	248	ILE	3.5
1	E	306	SER	3.5
1	A	89	LEU	3.5
1	B	398	LYS	3.5
1	D	97	SER	3.5
1	E	310	SER	3.5
1	E	37	ALA	3.5
1	F	452	TYR	3.5
1	D	266	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	120	VAL	3.5
1	F	417	HIS	3.5
1	C	156	ILE	3.5
1	C	41	LYS	3.5
1	F	18	ASN	3.4
1	D	208	GLY	3.4
1	F	56	GLY	3.4
1	F	346	GLY	3.4
1	E	105	LEU	3.4
1	C	166	GLU	3.4
1	E	295	LYS	3.4
1	F	47	HIS	3.4
1	E	232	GLY	3.4
1	C	225	ASP	3.4
1	E	436	PRO	3.4
1	E	402	ILE	3.4
1	B	210	VAL	3.4
1	B	419	VAL	3.4
1	C	31	ASN	3.4
1	D	135	LYS	3.4
1	F	133	ASP	3.4
1	B	447	CYS	3.4
1	E	20	ASN	3.4
1	F	334	GLU	3.4
1	F	163	HIS	3.4
1	D	375	GLY	3.4
1	D	403	SER	3.4
1	C	348	ILE	3.4
1	E	245	ALA	3.4
1	C	10	GLU	3.4
1	D	262	VAL	3.4
1	F	25	GLY	3.4
1	D	68	ASP	3.4
1	A	108	LEU	3.4
1	D	171	HIS	3.4
1	A	234	ASN	3.4
1	C	447	CYS	3.4
1	E	192	ASP	3.4
1	D	4	ARG	3.4
1	F	429	ALA	3.4
1	E	491	VAL	3.4
1	B	223	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	394	PRO	3.3
1	F	324	PHE	3.3
1	F	237	ALA	3.3
1	F	476	PHE	3.3
1	E	131	THR	3.3
1	E	150	ARG	3.3
1	E	266	VAL	3.3
1	F	285	VAL	3.3
1	B	224	LEU	3.3
1	D	274	PRO	3.3
1	F	105	LEU	3.3
1	D	227	VAL	3.3
1	A	224	LEU	3.3
1	A	217	ASP	3.3
1	B	264	ASN	3.3
1	E	48	GLU	3.3
1	C	259	VAL	3.3
1	B	74	ALA	3.3
1	B	165	LYS	3.3
1	D	219	SER	3.3
1	F	231	ILE	3.3
1	E	117	TYR	3.3
1	D	202	ASP	3.3
1	D	230	ALA	3.3
1	B	167	ILE	3.3
1	F	390	ILE	3.3
1	B	70	VAL	3.3
1	B	130	VAL	3.3
1	D	177	LEU	3.3
1	F	430	ASP	3.3
1	D	44	ILE	3.3
1	E	183	ARG	3.2
1	F	256	GLN	3.2
1	B	265	ALA	3.2
1	F	319	ALA	3.2
1	C	402	ILE	3.2
1	A	448	VAL	3.2
1	D	70	VAL	3.2
1	E	448	VAL	3.2
1	F	142	VAL	3.2
1	A	190	PRO	3.2
1	B	465	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	93	ILE	3.2
1	C	127	VAL	3.2
1	E	138	PRO	3.2
1	A	102	ASP	3.2
1	E	272	ASP	3.2
1	F	490	ASN	3.2
1	F	340	GLU	3.2
1	B	336	SER	3.2
1	E	377	GLY	3.2
1	E	280	ASN	3.2
1	A	364	SER	3.2
1	C	379	SER	3.2
1	F	29	ALA	3.2
1	E	462	LEU	3.2
1	F	226	PRO	3.2
1	F	398	LYS	3.2
1	B	113	ARG	3.2
1	F	320	ASN	3.2
1	F	219	SER	3.2
1	B	139	THR	3.2
1	D	342	VAL	3.2
1	E	76	ALA	3.2
1	E	104	HIS	3.2
1	E	314	ILE	3.2
1	E	426	TRP	3.2
1	B	369	GLY	3.2
1	F	169	GLY	3.2
1	A	349	THR	3.2
1	B	269	ALA	3.2
1	B	429	ALA	3.2
1	A	460	LEU	3.1
1	D	299	ILE	3.1
1	F	55	ILE	3.1
1	D	351	ASN	3.1
1	B	427	GLY	3.1
1	D	353	ALA	3.1
1	E	3	LEU	3.1
1	E	341	ILE	3.1
1	E	496	TYR	3.1
1	A	436	PRO	3.1
1	C	77	VAL	3.1
1	C	409	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	149	CYS	3.1
1	E	263	ALA	3.1
1	F	153	ASP	3.1
1	E	317	ILE	3.1
1	E	190	PRO	3.1
1	F	297	GLY	3.1
1	B	131	THR	3.1
1	F	341	ILE	3.1
1	F	444	ILE	3.1
1	D	389	SER	3.1
1	F	262	VAL	3.1
1	F	303	SER	3.1
1	A	182	ARG	3.1
1	F	54	LYS	3.1
1	F	414	HIS	3.1
1	C	289	ALA	3.1
1	D	283	THR	3.1
1	E	112	LEU	3.1
1	F	137	LEU	3.1
1	F	345	LEU	3.1
1	B	402	ILE	3.1
1	D	348	ILE	3.1
1	C	26	PHE	3.1
1	C	265	ALA	3.1
1	E	11	ALA	3.1
1	A	255	LEU	3.1
1	B	258	GLY	3.1
1	D	169	GLY	3.1
1	F	118	GLY	3.1
1	F	162	LYS	3.1
1	E	308	SER	3.1
1	E	34	VAL	3.1
1	F	70	VAL	3.1
1	D	81	THR	3.1
1	E	292	ALA	3.1
1	D	92	LEU	3.1
1	D	108	LEU	3.1
1	F	211	ARG	3.1
1	F	239	LEU	3.1
1	F	258	GLY	3.1
1	A	79	PHE	3.1
1	C	324	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	387	TYR	3.1
1	E	45	ALA	3.0
1	F	5	PHE	3.0
1	A	357	ASP	3.0
1	B	87	LYS	3.0
1	F	298	ARG	3.0
1	B	471	ASN	3.0
1	E	270	LEU	3.0
1	F	385	ASN	3.0
1	E	480	GLN	3.0
1	B	21	VAL	3.0
1	B	195	GLY	3.0
1	C	237	ALA	3.0
1	F	466	GLY	3.0
1	E	478	PHE	3.0
1	F	116	PHE	3.0
1	B	227	VAL	3.0
1	F	34	VAL	3.0
1	F	343	ARG	3.0
1	D	134	GLY	3.0
1	B	462	LEU	3.0
1	F	456	LEU	3.0
1	C	277	PRO	3.0
1	F	413	ASP	3.0
1	C	18	ASN	3.0
1	C	208	GLY	3.0
1	F	218	GLU	3.0
1	E	139	THR	3.0
1	B	101	PHE	3.0
1	B	146	PRO	3.0
1	C	206	ILE	3.0
1	C	413	ASP	3.0
1	B	367	VAL	3.0
1	D	130	VAL	3.0
1	C	60	GLY	3.0
1	A	103	LEU	3.0
1	E	482	LEU	3.0
1	F	159	LEU	3.0
1	B	241	SER	3.0
1	B	424	SER	3.0
1	A	324	PHE	3.0
1	E	197	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	217	ASP	3.0
1	D	144	ILE	3.0
1	F	6	ILE	3.0
1	B	347	VAL	3.0
1	B	377	GLY	3.0
1	D	199	VAL	3.0
1	A	91	ASN	3.0
1	D	216	ASN	3.0
1	E	83	TYR	3.0
1	E	177	LEU	3.0
1	A	370	THR	3.0
1	D	42	ARG	3.0
1	D	306	SER	3.0
1	E	59	THR	3.0
1	F	24	SER	3.0
1	E	176	PRO	3.0
1	A	358	ILE	3.0
1	B	358	ILE	3.0
1	A	207	VAL	3.0
1	F	21	VAL	3.0
1	C	482	LEU	2.9
1	F	108	LEU	2.9
1	A	36	PRO	2.9
1	B	332	PRO	2.9
1	C	116	PHE	2.9
1	E	172	ASP	2.9
1	C	299	ILE	2.9
1	D	376	ILE	2.9
1	C	177	LEU	2.9
1	D	117	TYR	2.9
1	B	81	THR	2.9
1	A	23	PHE	2.9
1	E	25	GLY	2.9
1	E	291	ILE	2.9
1	E	371	ARG	2.9
1	D	462	LEU	2.9
1	D	98	THR	2.9
1	F	140	THR	2.9
1	F	468	THR	2.9
1	C	315	GLN	2.9
1	F	277	PRO	2.9
1	E	165	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	300	LYS	2.9
1	F	369	GLY	2.9
1	B	155	ILE	2.9
1	D	303	SER	2.9
1	E	106	SER	2.9
1	E	219	SER	2.9
1	E	251	ASP	2.9
1	F	129	ASP	2.9
1	C	378	GLY	2.9
1	E	146	PRO	2.9
1	E	55	ILE	2.9
1	E	348	ILE	2.9
1	E	475	CYS	2.9
1	E	367	VAL	2.9
1	E	241	SER	2.9
1	F	233	ASP	2.9
1	A	356	ALA	2.9
1	B	40	ALA	2.9
1	F	401	LYS	2.9
1	C	370	THR	2.9
1	D	59	THR	2.9
1	E	271	GLY	2.9
1	A	227	VAL	2.9
1	A	326	ASP	2.9
1	B	182	ARG	2.9
1	E	147	THR	2.9
1	F	53	PHE	2.9
1	E	167	ILE	2.9
1	A	293	LEU	2.9
1	C	256	GLN	2.9
1	E	130	VAL	2.9
1	F	347	VAL	2.9
1	B	29	ALA	2.9
1	D	436	PRO	2.9
1	B	6	ILE	2.8
1	B	239	LEU	2.8
1	F	106	SER	2.8
1	F	157	VAL	2.8
1	B	474	CYS	2.8
1	B	352	THR	2.8
1	E	244	LYS	2.8
1	F	301	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	467	GLN	2.8
1	B	317	ILE	2.8
1	A	262	VAL	2.8
1	E	330	LEU	2.8
1	E	403	SER	2.8
1	B	107	THR	2.8
1	C	471	ASN	2.8
1	B	461	GLU	2.8
1	C	306	SER	2.8
1	D	362	ILE	2.8
1	D	460	LEU	2.8
1	F	177	LEU	2.8
1	C	309	VAL	2.8
1	F	392	THR	2.8
1	A	58	PHE	2.8
1	E	320	ASN	2.8
1	E	476	PHE	2.8
1	E	193	ARG	2.8
1	F	461	GLU	2.8
1	E	282	TYR	2.8
1	A	167	ILE	2.8
1	A	219	SER	2.8
1	F	121	ASP	2.8
1	A	427	GLY	2.8
1	E	444	ILE	2.8
1	C	79	PHE	2.8
1	F	126	GLU	2.8
1	F	333	GLN	2.8
1	A	465	LYS	2.8
1	D	381	ASP	2.8
1	B	354	LEU	2.8
1	B	184	GLU	2.8
1	E	82	PRO	2.8
1	F	434	LYS	2.8
1	C	430	ASP	2.8
1	C	83	TYR	2.8
1	C	258	GLY	2.8
1	C	335	TYR	2.8
1	E	145	LEU	2.8
1	E	378	GLY	2.8
1	D	325	LYS	2.8
1	D	432	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	230	ALA	2.8
1	C	45	ALA	2.8
1	B	189	THR	2.8
1	D	364	SER	2.8
1	F	244	LYS	2.8
1	C	140	THR	2.8
1	C	147	THR	2.8
1	C	250	LYS	2.7
1	C	17	HIS	2.7
1	E	412	HIS	2.7
1	F	73	GLN	2.7
1	F	35	VAL	2.7
1	F	176	PRO	2.7
1	C	220	ASP	2.7
1	D	165	LYS	2.7
1	E	479	HIS	2.7
1	B	100	TYR	2.7
1	A	235	VAL	2.7
1	C	342	VAL	2.7
1	C	230	ALA	2.7
1	B	217	ASP	2.7
1	B	274	PRO	2.7
1	C	478	PHE	2.7
1	F	196	LYS	2.7
1	B	173	LEU	2.7
1	A	144	ILE	2.7
1	D	83	TYR	2.7
1	B	76	ALA	2.7
1	D	222	ALA	2.7
1	F	154	ARG	2.7
1	B	108	LEU	2.7
1	C	108	LEU	2.7
1	F	160	ASN	2.7
1	B	235	VAL	2.7
1	C	285	VAL	2.7
1	A	82	PRO	2.7
1	C	64	GLY	2.7
1	F	64	GLY	2.7
1	B	392	THR	2.7
1	C	303	SER	2.7
1	E	171	HIS	2.7
1	A	471	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	31	ASN	2.7
1	E	338	ASN	2.7
1	A	291	ILE	2.7
1	C	167	ILE	2.7
1	F	125	ILE	2.7
1	E	313	VAL	2.7
1	F	120	VAL	2.7
1	F	315	GLN	2.7
1	A	274	PRO	2.7
1	B	450	PRO	2.7
1	E	180	PRO	2.7
1	D	368	SER	2.7
1	F	293	LEU	2.7
1	A	218	GLU	2.7
1	B	174	CYS	2.7
1	D	340	GLU	2.7
1	F	51	ASN	2.7
1	C	73	GLN	2.7
1	C	248	ILE	2.7
1	D	124	ILE	2.7
1	B	309	VAL	2.7
1	D	232	GLY	2.7
1	D	341	ILE	2.7
1	D	387	TYR	2.7
1	B	325	LYS	2.7
1	B	460	LEU	2.7
1	C	431	LEU	2.7
1	C	234	ASN	2.7
1	F	31	ASN	2.7
1	A	136	ILE	2.7
1	D	192	ASP	2.7
1	E	44	ILE	2.7
1	E	369	GLY	2.7
1	E	406	VAL	2.7
1	E	459	TYR	2.7
1	F	419	VAL	2.7
1	B	152	ALA	2.7
1	E	40	ALA	2.7
1	D	158	GLU	2.7
1	C	185	LEU	2.6
1	C	330	LEU	2.6
1	E	137	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	344	ARG	2.6
1	A	251	ASP	2.6
1	F	487	ASP	2.6
1	A	342	VAL	2.6
1	B	248	ILE	2.6
1	B	262	VAL	2.6
1	C	117	TYR	2.6
1	F	312	SER	2.6
1	A	231	ILE	2.6
1	C	6	ILE	2.6
1	E	285	VAL	2.6
1	E	358	ILE	2.6
1	B	23	PHE	2.6
1	D	323	PHE	2.6
1	F	450	PRO	2.6
1	B	270	LEU	2.6
1	D	273	ASN	2.6
1	B	297	GLY	2.6
1	E	220	ASP	2.6
1	E	381	ASP	2.6
1	E	451	ASP	2.6
1	C	187	VAL	2.6
1	C	201	VAL	2.6
1	F	39	ILE	2.6
1	A	265	ALA	2.6
1	E	254	PRO	2.6
1	F	180	PRO	2.6
1	F	236	ALA	2.6
1	F	391	PHE	2.6
1	C	366	HIS	2.6
1	D	56	GLY	2.6
1	D	412	HIS	2.6
1	E	234	ASN	2.6
1	F	20	ASN	2.6
1	F	48	GLU	2.6
1	B	148	ILE	2.6
1	A	101	PHE	2.6
1	D	483	ALA	2.6
1	E	279	PHE	2.6
1	B	117	TYR	2.6
1	B	456	LEU	2.6
1	D	218	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	208	GLY	2.6
1	A	484	LYS	2.6
1	E	250	LYS	2.6
1	F	484	LYS	2.6
1	C	155	ILE	2.6
1	D	379	SER	2.6
1	F	135	LYS	2.6
1	B	201	VAL	2.6
1	C	341	ILE	2.6
1	E	187	VAL	2.6
1	F	186	PRO	2.6
1	A	282	TYR	2.6
1	B	435	ASN	2.6
1	C	375	GLY	2.6
1	C	171	HIS	2.6
1	D	479	HIS	2.6
1	A	84	GLN	2.6
1	E	325	LYS	2.6
1	B	324	PHE	2.6
1	C	394	PRO	2.6
1	E	39	ILE	2.6
1	D	45	ALA	2.5
1	A	112	LEU	2.5
1	B	89	LEU	2.5
1	A	233	ASP	2.5
1	B	320	ASN	2.5
1	C	383	THR	2.5
1	D	145	LEU	2.5
1	E	431	LEU	2.5
1	F	91	ASN	2.5
1	C	327	LYS	2.5
1	F	368	SER	2.5
1	A	201	VAL	2.5
1	C	125	ILE	2.5
1	A	61	ALA	2.5
1	C	134	GLY	2.5
1	E	440	ALA	2.5
1	A	383	THR	2.5
1	B	220	ASP	2.5
1	B	371	ARG	2.5
1	C	68	ASP	2.5
1	D	71	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	365	THR	2.5
1	D	104	HIS	2.5
1	E	366	HIS	2.5
1	F	198	TYR	2.5
1	A	156	ILE	2.5
1	B	240	VAL	2.5
1	E	433	GLY	2.5
1	A	267	LEU	2.5
1	C	42	ARG	2.5
1	E	86	ASN	2.5
1	F	222	ALA	2.5
1	E	87	LYS	2.5
1	A	301	PHE	2.5
1	D	197	PRO	2.5
1	B	288	ASP	2.5
1	B	291	ILE	2.5
1	B	362	ILE	2.5
1	C	361	ASN	2.5
1	C	484	LYS	2.5
1	D	240	VAL	2.5
1	E	4	ARG	2.5
1	E	155	ILE	2.5
1	F	109	ALA	2.5
1	F	220	ASP	2.5
1	E	284	GLU	2.5
1	F	191	SER	2.5
1	D	331	ARG	2.5
1	A	180	PRO	2.5
1	A	422	ILE	2.5
1	A	423	ILE	2.5
1	D	251	ASP	2.5
1	D	405	PHE	2.5
1	F	287	GLN	2.5
1	D	2	ALA	2.5
1	D	89	LEU	2.5
1	E	396	VAL	2.5
1	F	43	ALA	2.5
1	A	475	CYS	2.5
1	F	349	THR	2.5
1	A	165	LYS	2.5
1	F	87	LYS	2.5
1	C	143	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	315	GLN	2.5
1	A	320	ASN	2.5
1	B	338	ASN	2.5
1	C	301	PHE	2.5
1	A	388	VAL	2.5
1	B	285	VAL	2.5
1	B	422	ILE	2.5
1	D	402	ILE	2.5
1	E	417	HIS	2.5
1	A	193	ARG	2.5
1	F	113	ARG	2.5
1	F	415	SER	2.5
1	A	467	GLN	2.5
1	C	463	GLY	2.5
1	F	470	GLN	2.5
1	A	20	ASN	2.5
1	C	275	ASP	2.5
1	C	493	TRP	2.5
1	B	137	LEU	2.5
1	B	185	LEU	2.5
1	C	128	ALA	2.5
1	D	155	ILE	2.5
1	D	309	VAL	2.5
1	F	342	VAL	2.5
1	F	431	LEU	2.5
1	B	271	GLY	2.5
1	C	466	GLY	2.5
1	D	60	GLY	2.5
1	F	141	GLY	2.5
1	C	179	PRO	2.5
1	F	82	PRO	2.5
1	F	164	PRO	2.5
1	A	45	ALA	2.4
1	B	390	ILE	2.4
1	E	390	ILE	2.4
1	E	331	ARG	2.4
1	F	272	ASP	2.4
1	B	197	PRO	2.4
1	C	472	LEU	2.4
1	A	128	ALA	2.4
1	C	207	VAL	2.4
1	D	423	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	442	GLU	2.4
1	A	352	THR	2.4
1	D	311	ARG	2.4
1	A	35	VAL	2.4
1	C	276	ILE	2.4
1	E	135	LYS	2.4
1	E	133	ASP	2.4
1	B	374	ASN	2.4
1	C	371	ARG	2.4
1	D	9	GLU	2.4
1	E	384	ARG	2.4
1	A	419	VAL	2.4
1	C	240	VAL	2.4
1	A	360	GLY	2.4
1	D	54	LYS	2.4
1	B	283	THR	2.4
1	C	415	SER	2.4
1	D	189	THR	2.4
1	D	213	SER	2.4
1	D	424	SER	2.4
1	E	175	GLU	2.4
1	A	270	LEU	2.4
1	B	290	VAL	2.4
1	C	464	VAL	2.4
1	D	157	VAL	2.4
1	D	290	VAL	2.4
1	E	262	VAL	2.4
1	F	448	VAL	2.4
1	A	163	HIS	2.4
1	D	414	HIS	2.4
1	D	75	ASP	2.4
1	B	261	ASN	2.4
1	A	279	PHE	2.4
1	C	476	PHE	2.4
1	E	23	PHE	2.4
1	E	407	PRO	2.4
1	B	426	TRP	2.4
1	C	55	ILE	2.4
1	D	358	ILE	2.4
1	E	362	ILE	2.4
1	F	174	CYS	2.4
1	F	310	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	172	ASP	2.4
1	E	205	LYS	2.4
1	F	205	LYS	2.4
1	D	200	GLN	2.4
1	F	32	PRO	2.4
1	A	100	TYR	2.4
1	B	284	GLU	2.4
1	B	440	ALA	2.4
1	C	72	ALA	2.4
1	E	429	ALA	2.4
1	B	444	ILE	2.4
1	E	124	ILE	2.4
1	A	220	ASP	2.4
1	A	445	ASP	2.4
1	D	27	THR	2.4
1	E	484	LYS	2.4
1	A	31	ASN	2.4
1	D	480	GLN	2.4
1	C	5	PHE	2.3
1	C	82	PRO	2.3
1	C	382	PHE	2.3
1	C	353	ALA	2.3
1	E	122	VAL	2.3
1	F	302	ALA	2.3
1	A	283	THR	2.3
1	C	81	THR	2.3
1	E	96	GLY	2.3
1	E	158	GLU	2.3
1	E	195	GLY	2.3
1	C	300	LYS	2.3
1	A	114	TYR	2.3
1	A	303	SER	2.3
1	A	493	TRP	2.3
1	B	412	HIS	2.3
1	C	236	ALA	2.3
1	F	37	ALA	2.3
1	B	428	VAL	2.3
1	D	347	VAL	2.3
1	A	81	THR	2.3
1	A	362	ILE	2.3
1	F	98	THR	2.3
1	B	205	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	36	PRO	2.3
1	D	330	LEU	2.3
1	E	71	LEU	2.3
1	E	113	ARG	2.3
1	D	430	ASP	2.3
1	E	265	ALA	2.3
1	E	473	ASP	2.3
1	B	142	VAL	2.3
1	C	142	VAL	2.3
1	C	347	VAL	2.3
1	F	206	ILE	2.3
1	F	481	GLU	2.3
1	A	486	GLY	2.3
1	F	460	LEU	2.3
1	A	424	SER	2.3
1	C	241	SER	2.3
1	F	102	ASP	2.3
1	F	100	TYR	2.3
1	C	325	LYS	2.3
1	C	468	THR	2.3
1	C	494	GLU	2.3
1	E	439	ARG	2.3
1	E	463	GLY	2.3
1	F	463	GLY	2.3
1	E	267	LEU	2.3
1	A	305	CYS	2.3
1	B	68	ASP	2.3
1	B	135	LYS	2.3
1	D	250	LYS	2.3
1	B	280	ASN	2.3
1	F	406	VAL	2.3
1	C	59	THR	2.3
1	D	360	GLY	2.3
1	F	195	GLY	2.3
1	A	456	LEU	2.3
1	B	191	SER	2.3
1	E	404	SER	2.3
1	E	94	ASN	2.3
1	E	174	CYS	2.3
1	E	441	HIS	2.3
1	F	204	ALA	2.3
1	D	127	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	210	VAL	2.3
1	C	139	THR	2.3
1	E	22	GLY	2.3
1	F	352	THR	2.3
1	B	48	GLU	2.3
1	B	322	ASP	2.3
1	C	158	GLU	2.3
1	F	158	GLU	2.3
1	F	249	PRO	2.3
1	F	451	ASP	2.3
1	B	236	ALA	2.3
1	F	492	ARG	2.3
1	A	266	VAL	2.3
1	D	209	VAL	2.3
1	E	421	VAL	2.3
1	B	98	THR	2.3
1	C	282	TYR	2.3
1	A	325	LYS	2.3
1	F	425	GLU	2.2
1	C	197	PRO	2.2
1	C	217	ASP	2.2
1	E	58	PHE	2.2
1	D	415	SER	2.2
1	D	298	ARG	2.2
1	E	489	ARG	2.2
1	F	384	ARG	2.2
1	D	123	ALA	2.2
1	B	50	GLY	2.2
1	D	396	VAL	2.2
1	D	406	VAL	2.2
1	F	78	LYS	2.2
1	F	115	GLY	2.2
1	B	229	GLN	2.2
1	C	124	ILE	2.2
1	A	149	CYS	2.2
1	C	188	TYR	2.2
1	D	314	ILE	2.2
1	E	7	THR	2.2
1	E	443	ILE	2.2
1	F	393	THR	2.2
1	E	355	GLU	2.2
1	E	416	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	213	SER	2.2
1	E	97	SER	2.2
1	A	95	ASN	2.2
1	A	196	LYS	2.2
1	A	74	ALA	2.2
1	B	353	ALA	2.2
1	E	449	HIS	2.2
1	C	246	GLY	2.2
1	D	259	VAL	2.2
1	B	423	ILE	2.2
1	B	443	ILE	2.2
1	B	493	TRP	2.2
1	D	481	GLU	2.2
1	F	423	ILE	2.2
1	E	100	TYR	2.2
1	C	399	ASP	2.2
1	A	403	SER	2.2
1	B	405	PHE	2.2
1	D	62	SER	2.2
1	D	343	ARG	2.2
1	F	79	PHE	2.2
1	E	465	LYS	2.2
1	F	306	SER	2.2
1	B	216	ASN	2.2
1	A	204	ALA	2.2
1	B	232	GLY	2.2
1	F	171	HIS	2.2
1	A	157	VAL	2.2
1	B	259	VAL	2.2
1	A	124	ILE	2.2
1	A	155	ILE	2.2
1	B	83	TYR	2.2
1	B	114	TYR	2.2
1	B	211	ARG	2.2
1	D	288	ASP	2.2
1	E	316	ASP	2.2
1	F	111	ASP	2.2
1	A	404	SER	2.2
1	C	450	PRO	2.2
1	D	312	SER	2.2
1	F	339	PRO	2.2
1	F	474	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	374	ASN	2.2
1	A	169	GLY	2.2
1	A	366	HIS	2.2
1	E	56	GLY	2.2
1	E	494	GLU	2.2
1	A	269	ALA	2.2
1	C	356	ALA	2.2
1	D	484	LYS	2.2
1	E	493	TRP	2.2
1	E	274	PRO	2.2
1	E	391	PHE	2.2
1	B	61	ALA	2.2
1	C	446	LYS	2.2
1	E	70	VAL	2.2
1	A	350	ILE	2.2
1	B	206	ILE	2.2
1	B	482	LEU	2.2
1	C	192	ASP	2.2
1	E	283	THR	2.2
1	F	225	ASP	2.2
1	C	213	SER	2.2
1	C	485	SER	2.2
1	A	164	PRO	2.2
1	A	450	PRO	2.2
1	C	58	PHE	2.2
1	D	494	GLU	2.2
1	F	436	PRO	2.2
1	F	469	PRO	2.2
1	D	141	GLY	2.2
1	E	273	ASN	2.2
1	A	150	ARG	2.2
1	B	15	VAL	2.2
1	A	426	TRP	2.2
1	C	272	ASP	2.2
1	E	288	ASP	2.2
1	F	396	VAL	2.2
1	D	125	ILE	2.2
1	F	242	GLU	2.2
1	F	358	ILE	2.2
1	A	241	SER	2.2
1	B	219	SER	2.2
1	B	14	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	5	PHE	2.2
1	D	23	PHE	2.2
1	B	162	LYS	2.2
1	D	100	TYR	2.2
1	D	394	PRO	2.2
1	E	332	PRO	2.2
1	D	46	ALA	2.2
1	A	409	VAL	2.2
1	B	120	VAL	2.2
1	C	388	VAL	2.2
1	F	438	GLU	2.2
1	B	145	LEU	2.1
1	D	173	LEU	2.1
1	F	307	LEU	2.1
1	F	354	LEU	2.1
1	F	241	SER	2.1
1	F	364	SER	2.1
1	D	86	ASN	2.1
1	D	459	TYR	2.1
1	F	273	ASN	2.1
1	D	438	GLU	2.1
1	C	102	ASP	2.1
1	A	27	THR	2.1
1	A	140	THR	2.1
1	A	447	CYS	2.1
1	C	474	CYS	2.1
1	B	293	LEU	2.1
1	C	71	LEU	2.1
1	D	448	VAL	2.1
1	E	293	LEU	2.1
1	B	136	ILE	2.1
1	B	190	PRO	2.1
1	C	273	ASN	2.1
1	C	338	ASN	2.1
1	D	320	ASN	2.1
1	E	32	PRO	2.1
1	E	382	PHE	2.1
1	D	188	TYR	2.1
1	D	282	TYR	2.1
1	F	17	HIS	2.1
1	F	355	GLU	2.1
1	C	161	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	302	ALA	2.1
1	A	392	THR	2.1
1	C	393	THR	2.1
1	D	131	THR	2.1
1	F	145	LEU	2.1
1	A	44	ILE	2.1
1	A	50	GLY	2.1
1	B	144	ILE	2.1
1	E	299	ILE	2.1
1	C	221	PHE	2.1
1	E	374	ASN	2.1
1	F	86	ASN	2.1
1	C	414	HIS	2.1
1	A	68	ASP	2.1
1	B	487	ASP	2.1
1	E	430	ASP	2.1
1	D	85	SER	2.1
1	D	106	SER	2.1
1	D	107	THR	2.1
1	E	247	ARG	2.1
1	F	27	THR	2.1
1	F	453	ARG	2.1
1	B	39	ILE	2.1
1	B	86	ASN	2.1
1	C	443	ILE	2.1
1	E	490	ASN	2.1
1	C	359	PHE	2.1
1	E	339	PRO	2.1
1	E	495	ASP	2.1
1	C	46	ALA	2.1
1	A	377	GLY	2.1
1	C	97	SER	2.1
1	C	154	ARG	2.1
1	E	298	ARG	2.1
1	F	42	ARG	2.1
1	A	6	ILE	2.1
1	A	49	LYS	2.1
1	B	51	ASN	2.1
1	E	166	GLU	2.1
1	E	264	ASN	2.1
1	F	216	ASN	2.1
1	A	315	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	475	CYS	2.1
1	D	161	ASP	2.1
1	D	198	TYR	2.1
1	E	452	TYR	2.1
1	A	85	SER	2.1
1	A	306	SER	2.1
1	B	431	LEU	2.1
1	C	126	GLU	2.1
1	C	307	LEU	2.1
1	F	486	GLY	2.1
1	B	18	ASN	2.1
1	C	199	VAL	2.1
1	F	81	THR	2.1
1	A	148	ILE	2.1
1	A	317	ILE	2.1
1	A	348	ILE	2.1
1	B	44	ILE	2.1
1	B	252	PHE	2.1
1	F	279	PHE	2.1
1	E	357	ASP	2.1
1	C	483	ALA	2.1
1	E	74	ALA	2.1
1	E	126	GLU	2.1
1	E	356	ALA	2.1
1	C	364	SER	2.1
1	D	301	PHE	2.1
1	E	5	PHE	2.1
1	E	238	PHE	2.1
1	A	434	LYS	2.1
1	B	343	ARG	2.1
1	B	401	LYS	2.1
1	E	437	ARG	2.1
1	B	25	GLY	2.1
1	B	282	TYR	2.1
1	B	85	SER	2.1
1	D	109	ALA	2.1
1	D	482	LEU	2.0
1	A	94	ASN	2.0
1	A	361	ASN	2.0
1	C	91	ASN	2.0
1	A	142	VAL	2.0
1	B	207	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	406	VAL	2.0
1	B	468	THR	2.0
1	E	342	VAL	2.0
1	F	139	THR	2.0
1	B	299	ILE	2.0
1	C	362	ILE	2.0
1	E	359	PHE	2.0
1	A	133	ASP	2.0
1	A	225	ASP	2.0
1	C	311	ARG	2.0
1	D	439	ARG	2.0
1	E	80	ARG	2.0
1	B	496	TYR	2.0
1	F	265	ALA	2.0
1	A	145	LEU	2.0
1	B	177	LEU	2.0
1	B	307	LEU	2.0
1	B	351	ASN	2.0
1	D	105	LEU	2.0
1	E	239	LEU	2.0
1	A	210	VAL	2.0
1	B	33	LYS	2.0
1	B	187	VAL	2.0
1	C	283	THR	2.0
1	D	409	VAL	2.0
1	E	207	VAL	2.0
1	F	189	THR	2.0
1	D	382	PHE	2.0
1	E	215	PRO	2.0
1	E	343	ARG	2.0
1	B	172	ASP	2.0
1	C	152	ALA	2.0
1	D	265	ALA	2.0
1	A	139	THR	2.0
1	E	227	VAL	2.0
1	B	153	ASP	2.0
1	F	254	PRO	2.0
1	B	466	GLY	2.0
1	D	143	GLY	2.0
1	D	441	HIS	2.0
1	E	346	GLY	2.0
1	F	84	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	67	LEU	2.0
1	B	105	LEU	2.0
1	B	109	ALA	2.0
1	E	387	TYR	2.0
1	F	455	LEU	2.0
1	A	240	VAL	2.0
1	A	53	PHE	2.0
1	A	174	CYS	2.0
1	B	5	PHE	2.0
1	B	149	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	D	507	1/1	0.85	0.10	-3.35	17,17,17,17	0
2	ZN	E	507	1/1	0.97	0.07	-3.47	15,15,15,15	0
2	ZN	B	507	1/1	0.89	0.09	-4.15	20,20,20,20	0
2	ZN	C	507	1/1	0.94	0.10	-4.38	18,18,18,18	0
2	ZN	E	508	1/1	0.86	0.10	-5.67	25,25,25,25	0
2	ZN	A	507	1/1	0.87	0.09	-5.74	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.