



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:27 am BST

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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

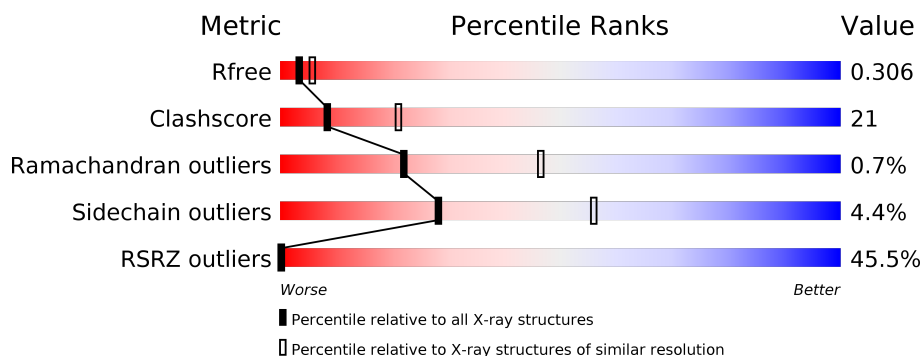
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	506	<div> <div>31%</div> <div>65%</div> <div>30%</div> <div>..</div> </div>
1	B	506	<div> <div>36%</div> <div>64%</div> <div>31%</div> <div>..</div> </div>
1	C	506	<div> <div>34%</div> <div>65%</div> <div>30%</div> <div>..</div> </div>
1	D	506	<div> <div>38%</div> <div>65%</div> <div>30%</div> <div>..</div> </div>
1	E	506	<div> <div>61%</div> <div>61%</div> <div>34%</div> <div>..</div> </div>
1	F	506	<div> <div>61%</div> <div>61%</div> <div>34%</div> <div>..</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
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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

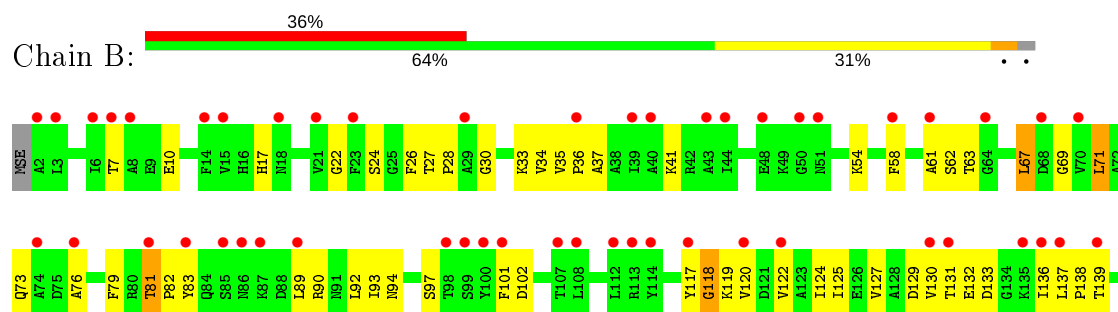
3 Residue-property plots

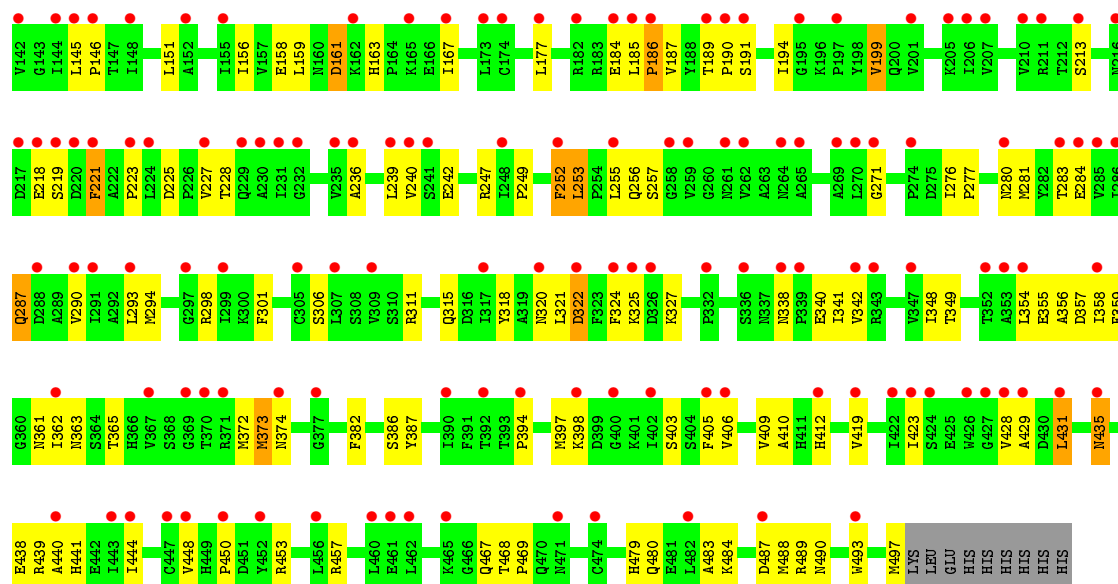
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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

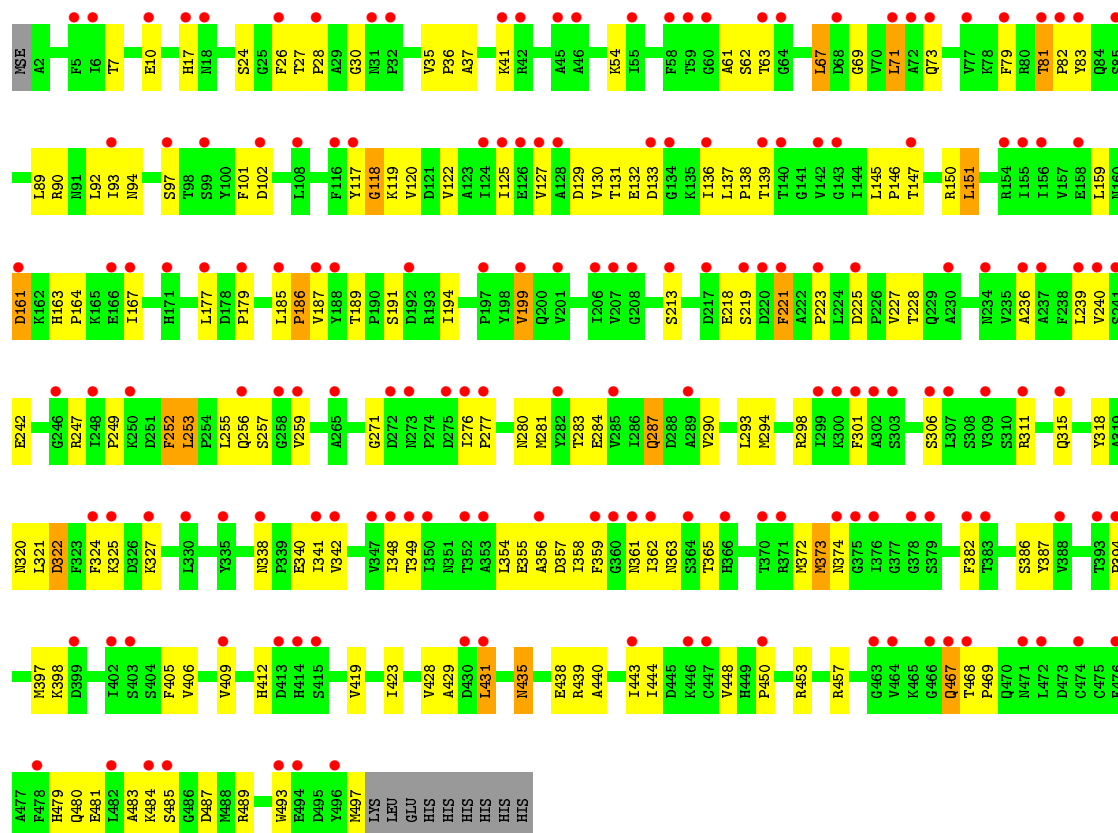


- Molecule 1: Acetyl-CoA hydrolase/transferase family protein

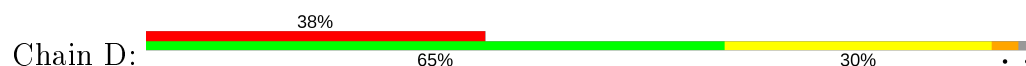


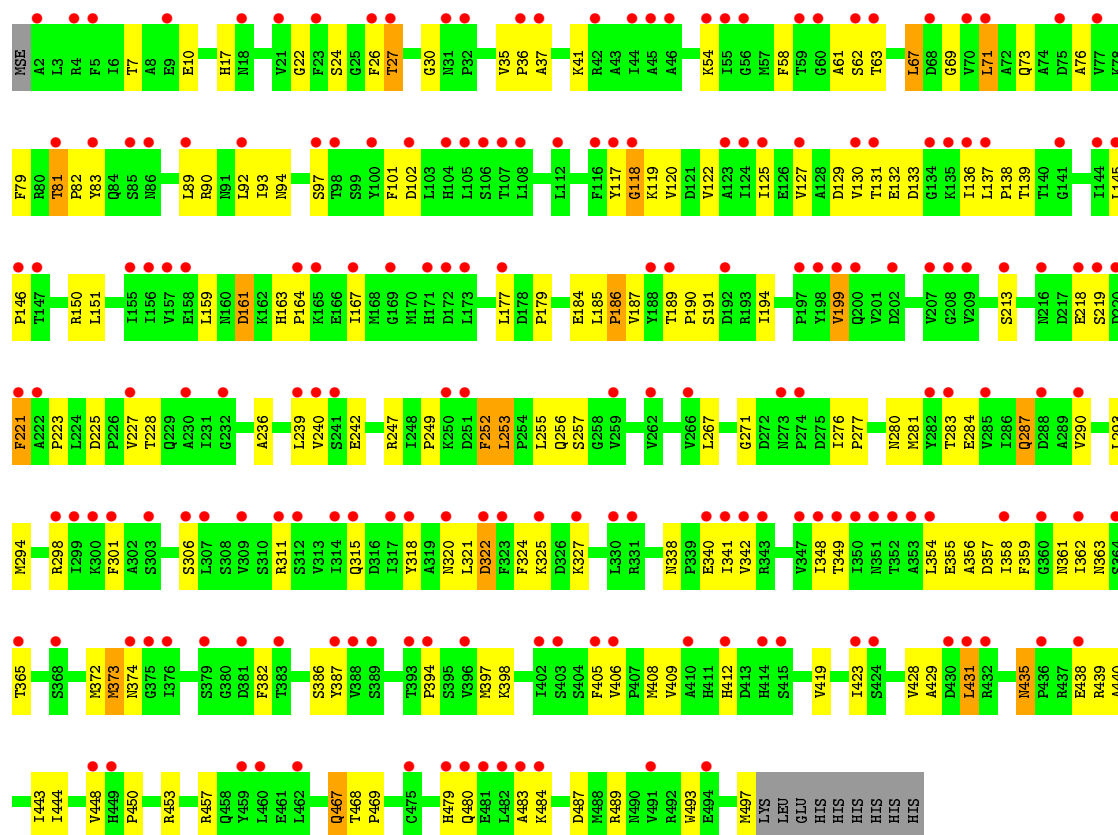


• Molecule 1: Acetyl-CoA hydrolase/transferase family protein

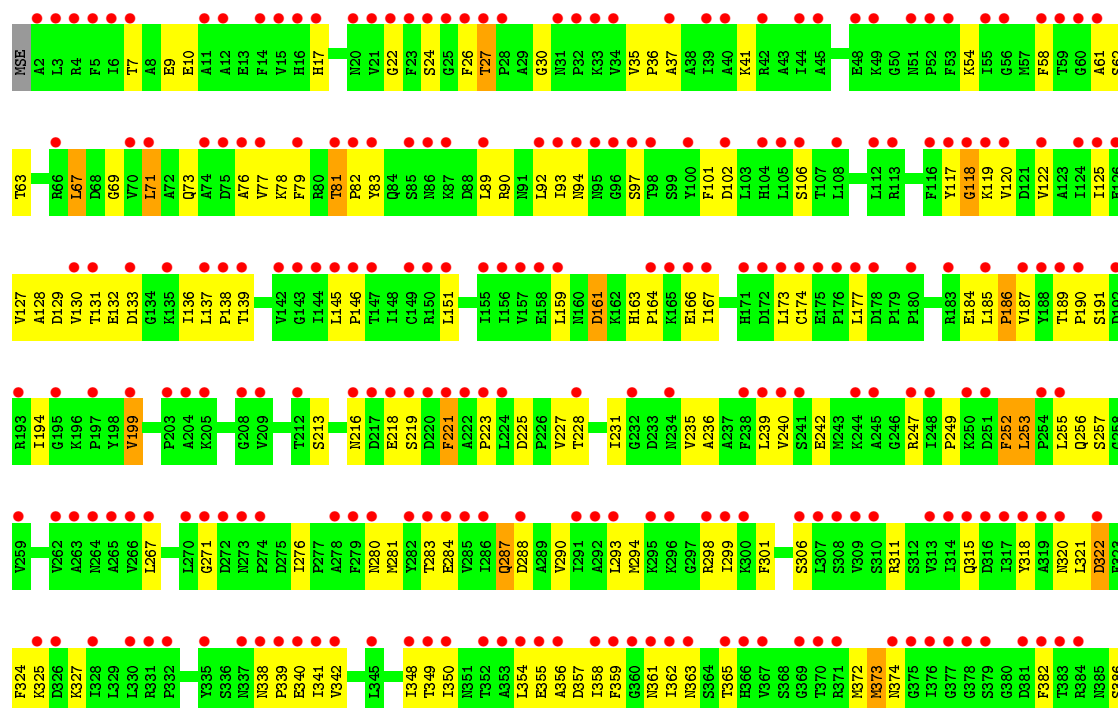


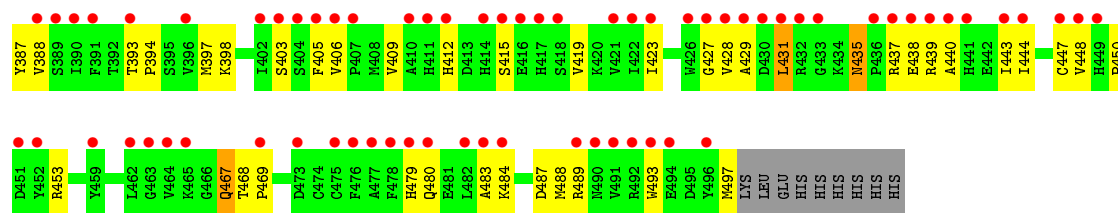
• Molecule 1: Acetyl-CoA hydrolase/transferase family protein



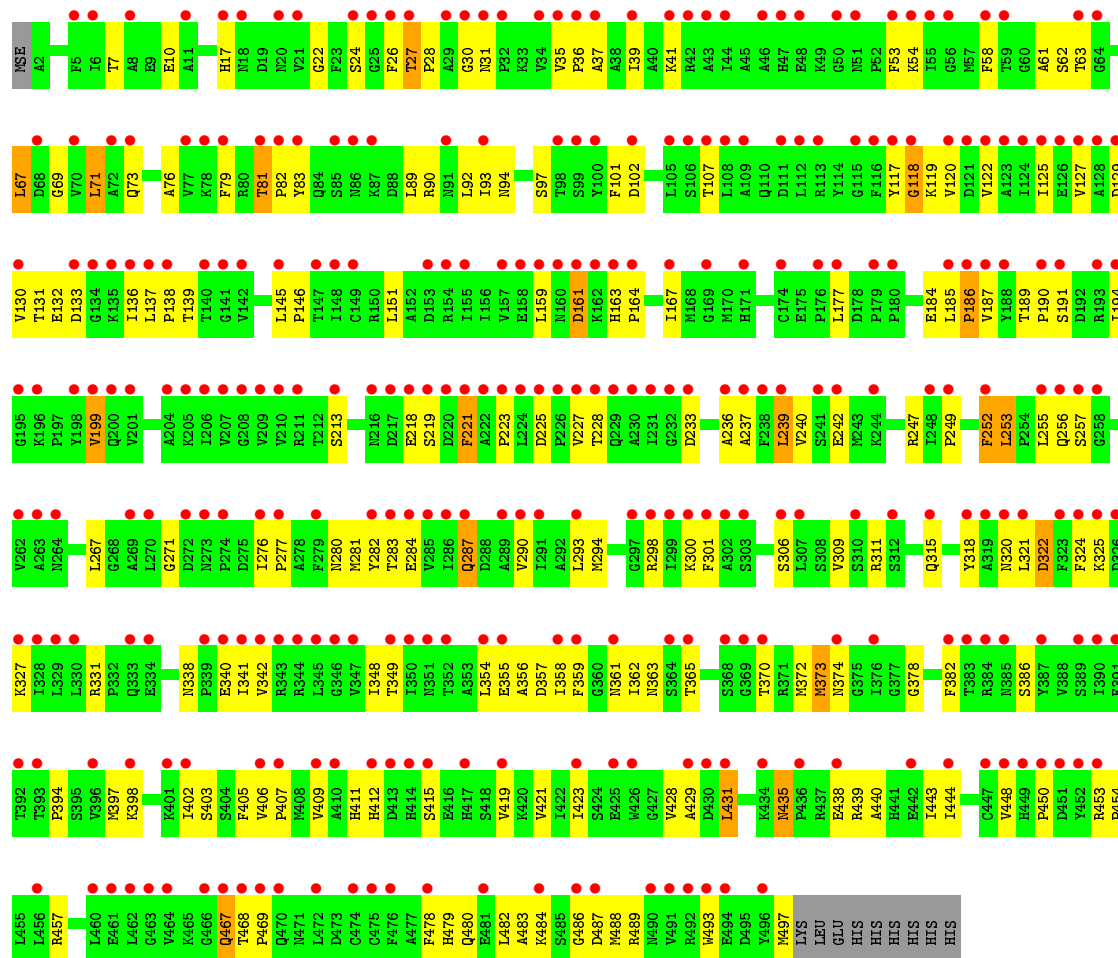


• Molecule 1: Acetyl-CoA hydrolase/transferase family protein





● 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	CNS 1.1, XTALVIEW	Depositor
R, R_{free}	0.287 , 0.290 0.307 , 0.306	Depositor DCC
R_{free} test set	8375 reflections (6.88%)	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	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
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, 0.333 respectively for untwinned datasets, and 0.375, 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:B:17:HIS:HD2	1:B:54:LYS:H	1.26	0.84
1:C:365:THR:O	1:C:373:MSE:HB2	1.78	0.84
1:A:365:THR:O	1:A:373:MSE:HB2	1.78	0.83
1:B:127:VAL:HG12	1:B:129:ASP:H	1.44	0.83
1:B:365:THR:O	1:B:373:MSE:HB2	1.77	0.83
1:E:127:VAL:HG12	1:E:129:ASP:H	1.43	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:A:480:GLN:O	1:A:484:LYS:HG2	1.79	0.82
1:C:17:HIS:HD2	1:C:54:LYS:H	1.27	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:450:PRO:HA	1:B:453:ARG:HG3	1.65	0.78
1:B:480:GLN:O	1:B:484:LYS:HG2	1.81	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:D:294:MSE:HE3	1:D:327:LYS:HB2	1.66	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
1:B:127:VAL:HG12	1:B:129:ASP:N	2.01	0.76
1:A:256:GLN:HA	1:A:283:THR:HG22	1.68	0.76
1:F:127:VAL:HG12	1:F:129:ASP:N	2.01	0.76
1:A:493:TRP:O	1:A:497:MSE:HG2	1.86	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: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: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:E:127:VAL:HG12	1:E:129:ASP:N	2.01	0.75
1:B:256:GLN:HA	1:B:283:THR:HG22	1.69	0.75
1:B:493:TRP:O	1:B:497:MSE:HG2	1.87	0.74
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: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:C:293:LEU:HD22	1:C:298:ARG:HG2	1.72	0.71
1:D:435:ASN:ND2	1:D:438:GLU:H	1.88	0.71
1:B:435:ASN:HD21	1:B:438:GLU:HG3	1.54	0.71
1:E:106:SER:HB2	3:E:554:HOH:O	1.91	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:B:479:HIS:NE2	3:B:524:HOH:O	2.23	0.70
1:D:435:ASN:HD21	1:D:438:GLU:HG3	1.56	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:A:435:ASN:HD21	1:A:438:GLU:HG3	1.58	0.67
1:D:349:THR:HG21	1:D:382:PHE:HB3	1.76	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:164:PRO:HG2	3:F:544:HOH:O	1.93	0.67
1:F:349:THR:HG21	1:F:382:PHE:HB3	1.76	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:C:187:VAL:HG13	1:C:341:ILE:HD12	1.76	0.66
1:E:435:ASN:ND2	1:E:438:GLU:H	1.92	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:190:PRO:HB2	3:F:545:HOH:O	1.96	0.65
1:F:294:MSE:HE3	1:F:327:LYS:CB	2.26	0.65
1:A:81:THR:HG23	1:A:101:PHE:O	1.97	0.64
1:E:256:GLN:HA	1:E:283:THR:HG23	1.78	0.64
1:B:187:VAL:HG13	1:B:341:ILE:HD12	1.79	0.64
1:B:483:ALA:HB3	1:B:484:LYS:HE3	1.78	0.64
1:D:311:ARG:O	1:D:315:GLN:HG3	1.97	0.64
1:E:7:THR:OG1	1:E:10:GLU: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:C:435:ASN:HD21	1:C:438:GLU:H	1.44	0.64
1:D:294:MSE:HE3	1:D:327:LYS:CB	2.27	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: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: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:A:184:GLU:HG3	1:B:184:GLU:HG3	1.80	0.64
1:D:435:ASN:HD21	1:D:438:GLU:H	1.46	0.64
1:D:355:GLU:HG2	1:D:363:ASN:HB3	1.79	0.64
1:F:355:GLU:HG2	1:F:363:ASN:HB3	1.78	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:A:26:PHE:HB3	1:A:306:SER:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:GLU:HG2	1:B:363:ASN:HB3	1.78	0.63
1:D:294:MSE:HE2	1:D:324:PHE:CD2	2.34	0.63
1:A:483:ALA:HB3	1:A:484:LYS:HE3	1.80	0.63
1:E:127:VAL:CG1	1:E:129:ASP:H	2.12	0.63
1:B:287:GLN:HE21	1:B:287:GLN:H	1.46	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: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:A:294:MSE:HE3	1:A:327:LYS:CB	2.29	0.62
1:E:81:THR:HG23	1:E:101:PHE:O	1.99	0.62
1:A:355:GLU:HG2	1:A:363:ASN:HB3	1.81	0.62
1:C:119:LYS:HG2	1:C:120:VAL:N	2.14	0.62
1:F:457:ARG:NH2	3:F:515:HOH:O	2.32	0.62
1:A:186:PRO:HB2	3:A:512:HOH:O	2.00	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: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:A:119:LYS:HG2	1:A:120:VAL:N	2.14	0.62
1:B:187:VAL:CG1	1:B:341:ILE:HD12	2.30	0.62
1:C:189:THR:HG22	1:C:191:SER:H	1.65	0.62
1:C:167:ILE:HD11	1:C:318:TYR:CE2	2.34	0.62
1:D:187:VAL:CG1	1:D:341:ILE:HD12	2.30	0.62
1:D:483:ALA:HB3	1:D:484:LYS:HE3	1.82	0.62
1:E:167:ILE:HD11	1:E:318:TYR:CE2	2.35	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:A:287:GLN:H	1:A:287:GLN:HE21	1.48	0.61
1:A:435:ASN:HD21	1:A:438:GLU:H	1.47	0.61
1:B:294:MSE:HE2	1:B:324:PHE:CD2	2.34	0.61
1:E:435:ASN:HD21	1:E:438:GLU:H	1.48	0.61
1:B:119:LYS:HG2	1:B:120:VAL:N	2.14	0.61
1:E:311:ARG:O	1:E:315:GLN:HG3	2.00	0.61
1:F:411:HIS:HA	3:F:523:HOH:O	1.99	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:D:287:GLN:HE21	1:D:287:GLN:H	1.49	0.61
1:E:119:LYS:HG2	1:E:120:VAL:N	2.13	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:D:167:ILE:HD11	1:D:318:TYR:CE2	2.35	0.61
1:F:483:ALA:HB3	1:F:484:LYS:HE3	1.82	0.61
1:B:412:HIS:CD2	3:B:512:HOH:O	2.52	0.61
1:B:167:ILE:HD11	1:B:318:TYR:CE2	2.36	0.61
1:C:294:MSE:HE2	1:C:324:PHE:CD2	2.35	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:287:GLN:H	1:C:287:GLN:HE21	1.49	0.60
1:C:94:ASN:HD21	1:C:372:MSE:N	1.94	0.60
1:D:189:THR:HG22	1:D:191:SER:H	1.66	0.60
1:D:256:GLN:HA	1:D:283:THR:HG23	1.82	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:A:167:ILE:HD11	1:A:318:TYR:CE2	2.36	0.60
1:F:187:VAL:HG13	1:F:341:ILE:HD12	1.82	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:454:PRO:HG2	3:F:513:HOH:O	2.02	0.59
1:F:94:ASN:HD21	1:F:372:MSE:N	1.96	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:257:SER:H	1:F:283:THR:HG22	1.67	0.59
1:F:187:VAL:CG1	1:F:341:ILE:HD12	2.33	0.59
1:E:483:ALA:HB3	1:E:484:LYS:HE3	1.84	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: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: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: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:B:362:ILE:HD13	1:B:419:VAL:HG21	1.86	0.58
1:B:82:PRO:O	1:B:102:ASP:HA	2.02	0.58
1:C:448:VAL:O	1:C:453:ARG:HD3	2.02	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:A:311:ARG:O	1:A:315:GLN:HG3	2.04	0.58
1:B:287:GLN:NE2	1:B:287:GLN:H	2.02	0.58
1:F:435:ASN:HD21	1:F:438:GLU:H	1.50	0.58
1:B:435:ASN:HD22	1:B:435:ASN:C	2.07	0.58
1:F:421:VAL:HG13	3:F:514:HOH:O	2.04	0.58
1:A:82:PRO:O	1:A:102:ASP:HA	2.04	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:287:GLN:HB3	3:C:516:HOH:O	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:C:249:PRO:HG2	1:C:253:LEU:HD13	1.86	0.56
1:C:311:ARG:O	1:C:315:GLN:HG3	2.04	0.56
1:E:185:LEU:HB2	1:E:341:ILE:HD11	1.88	0.56
1:A:435:ASN:C	1:A:435:ASN:HD22	2.07	0.56
1:B:225:ASP:OD2	1:B:228:THR:HG23	2.05	0.56
1:E:435:ASN:C	1:E:435:ASN:HD22	2.09	0.56
1:B:90:ARG:HD3	1:B:373:MSE:O	2.05	0.56
1:E:358:ILE:O	1:E:440:ALA:HA	2.06	0.56
1:F:90:ARG:HD3	1:F:373:MSE:O	2.04	0.56
1:B:117:TYR:O	1:B:118:GLY:O	2.24	0.56
1:B:94:ASN:HD21	1:B:372:MSE:N	1.98	0.56
1:E:90:ARG:HD3	1:E:373:MSE:O	2.05	0.56
1:C:82:PRO:O	1:C:102:ASP:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:SER:H	1:E:283:THR:HG22	1.70	0.56
1:F:233:ASP:HB3	3:F:530:HOH:O	2.05	0.56
1:F:435:ASN:HD22	1:F:435:ASN:C	2.08	0.56
1:C:487:ASP:OD1	1:C:489:ARG:HD3	2.05	0.56
1:F:225:ASP:OD2	1:F:228:THR:HG23	2.06	0.56
1:C:218:GLU:HG3	1:C:219:SER:N	2.21	0.56
1:F:185:LEU:HB2	1:F:341:ILE:HD11	1.87	0.56
1:F:448:VAL:O	1:F: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:E:448:VAL:O	1:E:453:ARG:HD3	2.06	0.55
1:A:185:LEU:HB2	1:A:341:ILE:HD11	1.88	0.55
1:D:257:SER:H	1:D:283:THR:HG22	1.70	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:E:225:ASP:OD2	1:E:228:THR:HG23	2.06	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:D:185:LEU:HB2	1:D:341:ILE:HD11	1.89	0.55
1:E:36:PRO:HG3	1:E:67:LEU:HD22	1.88	0.55
1:F:349:THR:HG23	1:F:386:SER:HB3	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:A:218:GLU:HG3	1:A:219:SER:N	2.22	0.55
1:A:359:PHE:O	1:A:439:ARG:HD2	2.06	0.55
1:C:225:ASP:OD2	1:C:228:THR:HG23	2.07	0.55
1:C:185:LEU:HB2	1:C:341:ILE:HD11	1.88	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: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:90:ARG:HD3	1:D:373:MSE:O	2.06	0.54
1:D:358:ILE:O	1:D:440:ALA:HA	2.08	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:C:387:TYR:HE2	1:D:179:PRO:HG2	1.73	0.54
1:D:435:ASN:HD22	1:D:435:ASN:C	2.09	0.54
1:E:216:ASN:ND2	3:E:538:HOH:O	2.40	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: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:F:81:THR:HG22	1:F:82:PRO:CA	2.36	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:D:362:ILE:HD13	1:D:419:VAL:HG21	1.90	0.54
1:F:287:GLN:NE2	1:F:290:VAL:HG23	2.23	0.54
1:B:358:ILE:O	1:B:440:ALA:HA	2.07	0.54
1:C:90:ARG:HD3	1:C:373:MSE:O	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:A:92:LEU:HD12	1:A:97:SER:HB2	1.90	0.54
1:B:487:ASP:OD1	1:B:489:ARG:HD3	2.07	0.54
1:C:349:THR:HG23	1:C:386:SER:HB3	1.90	0.54
1:D:359:PHE:O	1:D:439:ARG:HD2	2.07	0.54
1:F:309:VAL:HA	3:F:525:HOH:O	2.08	0.54
1:F:435:ASN:ND2	1:F:438:GLU:HG3	2.21	0.54
1:B:257:SER:H	1:B:283:THR:HG22	1.72	0.54
1:D:130:VAL:O	1:D:130:VAL:HG13	2.08	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: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:D:117:TYR:O	1:D:118:GLY:O	2.27	0.53
1:D:287:GLN:NE2	1:D:287:GLN:H	2.07	0.53
1:E:287:GLN:H	1:E:287:GLN:NE2	2.06	0.53
1:C:117:TYR:O	1:C:118:GLY:O	2.27	0.53
1:D:225:ASP:OD2	1:D:228:THR:HG23	2.08	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:B:161:ASP:HB2	1:B:213:SER:HA	1.91	0.53
1:E:435:ASN:ND2	1:E:438:GLU:HG3	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ASP:HB2	1:D:213:SER:HA	1.90	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:E:30:GLY:HA2	1:E:139:THR:OG1	2.07	0.53
1:F:362:ILE:HD13	1:F:419:VAL:HG21	1.91	0.53
1:B:130:VAL:O	1:B:130:VAL:HG13	2.09	0.53
1:F:440:ALA:O	1:F:444:ILE:HG13	2.08	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:A:280:ASN:ND2	1:A:301:PHE:HB3	2.24	0.52
1:B:30:GLY:HA2	1:B:139:THR:OG1	2.08	0.52
1:C:81:THR:HG22	1:C:82:PRO:CA	2.37	0.52
1:D:30:GLY:HA2	1:D:139:THR:OG1	2.09	0.52
1:E:355:GLU:OE1	1:E:479:HIS:HE1	1.92	0.52
1:E:415:SER:HB2	3:F:541:HOH:O	2.09	0.52
1:F:287:GLN:HE21	1:F:287:GLN:H	1.55	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:C:30:GLY:HA2	1:C:139:THR:OG1	2.09	0.52
1:F:331:ARG:NH1	3:F:527:HOH:O	2.43	0.52
1:A:81:THR:HG22	1:A:82:PRO:CA	2.37	0.52
1:D:218:GLU:HG3	1:D:219:SER:N	2.25	0.52
1:E:340:GLU:CG	1:F:340:GLU:HG3	2.37	0.52
1:B:17:HIS:HD2	1:B:54:LYS:N	2.03	0.52
1:D:320:ASN:HA	1:D:322:ASP:OD1	2.09	0.52
1:E:77:VAL:HA	3:E:555:HOH:O	2.09	0.52
1:C:161:ASP:HB2	1:C:213:SER:HA	1.92	0.52
1:F:287:GLN:NE2	1:F:287:GLN:H	2.08	0.52
1:A:161:ASP:HB2	1:A:213:SER:HA	1.92	0.52
1:E:294:MSE:CE	1:E:327:LYS:HB2	2.38	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:C:36:PRO:HG3	1:C:67:LEU:HD22	1.92	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:320:ASN:HA	1:F:322:ASP:OD1	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:THR:HG22	1:B:82:PRO:CA	2.39	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: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:D:36:PRO:HG3	1:D:67:LEU:HD22	1.91	0.51
1:F:131:THR:CG2	1:F:133:ASP:OD1	2.58	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:271:GLY:HA2	1:D:298:ARG:HD2	1.93	0.51
1:D:81:THR:CG2	1:D:82:PRO:HA	2.38	0.51
1:F:281:MSE:HE3	1:F:283:THR:CG2	2.40	0.51
1:C:338:ASN:O	1:C:342:VAL:HG23	2.11	0.51
1:F:453:ARG:HD2	3:F:515:HOH:O	2.09	0.51
1:B:280:ASN:ND2	1:B:301:PHE:HB3	2.26	0.51
1:E:218:GLU:HG3	1:E:219:SER:N	2.26	0.51
1:E:349:THR:CG2	1:E:386:SER:HB3	2.41	0.51
1:C:280:ASN:ND2	1:C:301:PHE:HB3	2.26	0.50
1:D:294:MSE:CE	1:D:327:LYS:HB2	2.36	0.50
1:B:255:LEU:HD23	1:B:348:ILE:HB	1.93	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: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: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: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:E:340:GLU:HG3	1:F:340:GLU:CG	2.38	0.50
1:F:358:ILE:O	1:F:440:ALA:HA	2.10	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:B:320:ASN:HA	1:B:322:ASP:OD1	2.11	0.50
1:E:435:ASN:ND2	1:E:435:ASN:C	2.65	0.50
1:A:131:THR:HG22	1:A:132:GLU:N	2.27	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: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

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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:E:130:VAL:O	1:E:130:VAL: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: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:F:421:VAL:N	3:F:517:HOH:O	2.45	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: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:E:448:VAL:HG23	3:E:541:HOH:O	2.12	0.49
1:F:255:LEU:HD23	1:F:348:ILE:HB	1.94	0.49
1:C:130:VAL:HG13	1:C:130:VAL:O	2.13	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: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:E:349:THR:CG2	1:E:382:PHE:HB3	2.42	0.49
1:C:138:PRO:HG3	1:C:145:LEU:CD2	2.43	0.49
1:F:67:LEU:O	1:F:71:LEU:HB2	2.13	0.49
1:A:454:PRO:HG2	3:A:531:HOH:O	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:F:429:ALA:O	1:F:431:LEU:HD13	2.12	0.49
1:A:338:ASN:O	1:A:342:VAL:HG23	2.13	0.49
1:B:349:THR:CG2	1:B:386:SER:HB3	2.43	0.49
1:C:81:THR:CG2	1:C:82:PRO:HA	2.39	0.49
1:E:429:ALA:O	1:E:431:LEU:HD13	2.13	0.49
1:E:92:LEU:HD12	1:E:97:SER:HB2	1.95	0.49
1:F:130:VAL:O	1:F:130:VAL:HG13	2.13	0.49
1:F:331:ARG:HB3	3:F:537:HOH:O	2.12	0.49
1:A:138:PRO:HG3	1:A:145:LEU:CD2	2.43	0.49
1:C:354:LEU:HD11	1:C:373:MSE:HG3	1.95	0.49
1:C:435:ASN:ND2	1:C:438:GLU:HG3	2.26	0.49
1:D:435:ASN:ND2	1:D:435:ASN:C	2.66	0.49
1:A:280:ASN:HD22	1:A:301:PHE:HB3	1.78	0.49
1:E:280:ASN:ND2	1:E:301:PHE:HB3	2.28	0.49
1:E:435:ASN:ND2	1:E:438:GLU:CG	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:MSE:HG2	1:A:398:LYS:N	2.28	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:F:271:GLY:HA2	1:F:298:ARG:HD2	1.94	0.48
1:B:131:THR:HG22	1:B:132:GLU:N	2.29	0.48
1:B:35:VAL:N	1:B:36:PRO:HD2	2.29	0.48
1:C:340:GLU:HG3	1:D:340:GLU:CG	2.41	0.48
1:D:349:THR:CG2	1:D:382:PHE:HB3	2.43	0.48
1:E:221:PHE:CD1	1:E:223:PRO:HD3	2.47	0.48
1:A:294:MSE:CE	1:A:327:LYS:HB2	2.40	0.48
1:B:361:ASN:C	1:B:362:ILE:HD12	2.33	0.48
1:C:94:ASN:ND2	1:C:372:MSE:H	1.99	0.48
1:D:318:TYR:HA	1:D:321:LEU:CD1	2.43	0.48
1:D:349:THR:CG2	1:D:386:SER:HB3	2.44	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: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:349:THR:CG2	1:C:382:PHE:HB3	2.41	0.48
1:C:69:GLY:O	1:C:73:GLN:HG3	2.13	0.48
1:F:435:ASN:ND2	1:F:435:ASN:C	2.66	0.48
1:A:271:GLY:HA2	1:A:298:ARG:HD2	1.94	0.48
1:D:138:PRO:HG3	1:D:145:LEU:CD2	2.44	0.48
1:F:280:ASN:ND2	1:F:301:PHE:HB3	2.29	0.48
1:A:293:LEU:O	1:A:298:ARG:HB3	2.14	0.48
1:C:429:ALA:O	1:C:431:LEU:HD13	2.13	0.48
1:E:271:GLY:HA2	1:E:298:ARG:HD2	1.96	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:B:318:TYR:HA	1:B:321:LEU:CD1	2.43	0.48
1:B:423:ILE:HG12	1:B:428:VAL:HB	1.96	0.48
1:D:17:HIS:HD2	1:D:54:LYS:N	2.03	0.48
1:D:280:ASN:HD22	1:D:301:PHE:HB3	1.78	0.48
1:D:69:GLY:O	1:D:73:GLN:HG3	2.14	0.48
1:A:349:THR:CG2	1:A:386:SER:HB3	2.43	0.48
1:A:429:ALA:O	1:A:431:LEU:HD13	2.13	0.48
1:B:33:LYS:N	3:B:513:HOH:O	2.45	0.48
1:C:355:GLU:OE1	1:C:479:HIS:HE1	1.96	0.48
1:F:349:THR:CG2	1:F:382:PHE:HB3	2.42	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:A:69:GLY:O	1:A:73:GLN:HG3	2.14	0.48
1:C:349:THR:CG2	1:C:386:SER:HB3	2.44	0.48
1:C:89:LEU:O	1:C:93:ILE:HG13	2.13	0.48
1:D:131:THR:HG22	1:D:132:GLU:N	2.29	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: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:94:ASN:HD22	1:D:467:GLN:H	1.61	0.47
1:A:320:ASN:HA	1:A:322:ASP:OD1	2.14	0.47
1:C:131:THR:CG2	1:C:133:ASP:OD1	2.63	0.47
1:B:27:THR:HA	1:B:62:SER:OG	2.14	0.47
1:B:280:ASN:HD22	1:B:301:PHE:HB3	1.79	0.47
1:C:340:GLU:CG	1:D:340:GLU:HG3	2.42	0.47
1:E:221:PHE:CZ	1:E:223:PRO:HG3	2.50	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: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:B:281:MSE:HE3	1:B:283:THR:CG2	2.44	0.47
1:B:89:LEU:O	1:B:93:ILE:HG13	2.14	0.47
1:C:281:MSE:HE3	1:C:283:THR:HG23	1.96	0.47
1:C:294:MSE:CE	1:C:327:LYS:HB2	2.39	0.47
1:D:256:GLN:HG3	1:D:382:PHE:CE1	2.49	0.47
1:E:301:PHE:N	3:E:556:HOH:O	2.47	0.47
1:F:287:GLN:HE21	1:F:290:VAL:HG23	1.80	0.47
1:F:294:MSE:CE	1:F:327:LYS:HB2	2.39	0.47
1:F:89:LEU:O	1:F:93:ILE:HG13	2.14	0.47
1:C:481:GLU:OE1	1:C:485:SER:OG	2.30	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: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:A:349:THR:CG2	1:A:382:PHE:HB3	2.44	0.47
1:B:349:THR:CG2	1:B:382:PHE:HB3	2.43	0.47
1:E:17:HIS:HD2	1:E:54:LYS:N	2.02	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:A:130:VAL:HG13	1:A:130:VAL:O	2.14	0.47
1:E:9:GLU:HB2	3:E:557:HOH:O	2.14	0.47
1:F:318:TYR:HA	1:F:321:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:435:ASN:HD21	1:F:438:GLU:CG	2.26	0.47
1:A:298:ARG:NE	3:A:516:HOH:O	2.16	0.47
1:C:186:PRO:HG2	1:C:194:ILE:CG2	2.45	0.47
1:E:318:TYR:HA	1:E:321:LEU:CD1	2.44	0.47
1:A:17:HIS:HD2	1:A:54:LYS:N	2.03	0.46
1:A:423:ILE:HG12	1:A:428:VAL:HB	1.98	0.46
1:D:186:PRO:HG2	1:D:194:ILE:CG2	2.45	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: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:F:79:PHE:C	1:F:79:PHE:CD1	2.89	0.46
1:A:26:PHE:CE1	1:A:61:ALA:HB2	2.51	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:B:69:GLY:O	1:B:73:GLN:HG3	2.15	0.46
1:C:280:ASN:HD22	1:C:301:PHE:HB3	1.80	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:F:271:GLY:HA2	1:F:298:ARG:CD	2.44	0.46
1:F:397:MSE:HG2	1:F:398:LYS:N	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:F:35:VAL:N	1:F:36:PRO:HD2	2.30	0.46
1:A:271:GLY:HA2	1:A:298:ARG:CD	2.45	0.46
1:B:236:ALA:O	1:B:240:VAL:HG13	2.15	0.46
1:B:271:GLY:HA2	1:B:298:ARG:HD2	1.96	0.46
1:D:276:ILE:O	1:D:298:ARG:NH1	2.48	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:E:281:MSE:HE3	1:E:283:THR:HG23	1.98	0.46
1:E:448:VAL:N	3:E:541:HOH:O	2.47	0.46
1:F:355:GLU:HG3	1:F:409:VAL:HG12	1.98	0.46
1:B:138:PRO:HG3	1:B:145:LEU:CD2	2.45	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: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:A:4:ARG:NH1	3:A:529:HOH:O	2.44	0.46
1:D:257:SER:H	1:D:283:THR:CG2	2.28	0.46
1:D:271:GLY:HA2	1:D:298:ARG:CD	2.46	0.46
1:D:54:LYS:HG2	1:D:76:ALA:HA	1.98	0.46
1:E:186:PRO:HG2	1:E:194:ILE:CG2	2.46	0.46
1:E:435:ASN:HD21	1:E:438:GLU:CG	2.23	0.46
1:F:221:PHE:CE1	1:F:223:PRO:HB3	2.51	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: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:E:467:GLN:H	1:F:94:ASN:HD22	1.63	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:37:ALA:O	1:B:41:LYS:HG2	2.16	0.45
1:B:441:HIS:HE1	3:B:516:HOH:O	1.98	0.45
1:C:397:MSE:HG2	1:C:398:LYS:N	2.31	0.45
1:A:92:LEU:CD1	1:A:97:SER:HB2	2.46	0.45
1:B:276:ILE:O	1:B:298:ARG:NH1	2.49	0.45
1:C:257:SER:H	1:C:283:THR:CG2	2.29	0.45
1:D:429:ALA:O	1:D:431:LEU:HD13	2.15	0.45
1:E:271:GLY:HA2	1:E:298:ARG:CD	2.45	0.45
1:E:403:SER:H	1:E:488:MSE:SE	2.49	0.45
1:E:67:LEU:O	1:E:71:LEU:HB2	2.16	0.45
1:E:94:ASN:HD22	1:F:467:GLN:H	1.62	0.45
1:F:221:PHE:CE1	1:F:223:PRO:HD3	2.51	0.45
1:F:26:PHE:CE1	1:F:61:ALA:HB2	2.50	0.45
1:B:429:ALA:O	1:B:431:LEU:HD13	2.15	0.45
1:B:435:ASN:ND2	1:B:438:GLU:CG	2.79	0.45
1:D:89:LEU:O	1:D:93:ILE:HG13	2.16	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:F:354:LEU:HD11	1:F:373:MSE:HG3	1.98	0.45
1:A:35:VAL:N	1:A:36:PRO:HD2	2.31	0.45
1:B:453:ARG:O	1:B:457:ARG:HG3	2.17	0.45
1:D:423:ILE:HG12	1:D:428:VAL:HB	1.99	0.45
1:E:26:PHE:CE1	1:E:61:ALA:HB2	2.51	0.45
1:F:321:LEU:O	1:F:325:LYS:HB2	2.16	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:321:LEU:O	1:E:325:LYS:HB2	2.16	0.45
1:E:354:LEU:HD11	1:E:373:MSE:HG3	1.98	0.45
1:E:423:ILE:HG12	1:E:428:VAL:HB	1.99	0.45
1:F:293:LEU:O	1:F:298:ARG:HB3	2.17	0.45
1:C:26:PHE:CE1	1:C:61:ALA:HB2	2.52	0.45
1:C:271:GLY:HA2	1:C:298:ARG:CD	2.47	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:A:361:ASN:C	1:A:362:ILE:HD12	2.38	0.45
1:C:83:TYR:CZ	1:C:374:ASN:HB3	2.52	0.45
1:D:435:ASN:ND2	1:D:438:GLU:CG	2.79	0.45
1:F:145:LEU:HB3	1:F:146:PRO:CD	2.47	0.45
1:A:287:GLN:NE2	1:A:290:VAL:HG23	2.32	0.44
1:B:221:PHE:CE1	1:B:223:PRO:HB3	2.52	0.44
1:C:467:GLN:H	1:D:94:ASN:ND2	2.15	0.44
1:D:26:PHE:CE1	1:D:61:ALA:HB2	2.52	0.44
1:F:318:TYR:HA	1:F:321:LEU:HD13	1.98	0.44
1:A:37:ALA:O	1:A:41:LYS:HG2	2.18	0.44
1:B:271:GLY:HA2	1:B:298:ARG:CD	2.47	0.44
1:B:287:GLN:NE2	1:B:290:VAL:HG23	2.32	0.44
1:D:67:LEU:O	1:D:71:LEU:HB2	2.17	0.44
1:E:138:PRO:HG3	1:E:145:LEU:HD21	1.98	0.44
1:E:256:GLN:HG3	1:E:382:PHE:CE1	2.52	0.44
1:F:486:GLY:N	3:F:531:HOH:O	2.50	0.44
1:A:79:PHE:C	1:A:79:PHE:CD1	2.91	0.44
1:D:221:PHE:CE1	1:D:223:PRO:HD3	2.52	0.44
1:D:37:ALA:O	1:D:41:LYS:HG2	2.17	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:242:GLU:OE2	1:D:247:ARG:NH2	2.50	0.44
1:A:27:THR:HA	1:A:62:SER:OG	2.17	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:E:287:GLN:NE2	1:E:290:VAL:HG23	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:GLU:HG3	1:F:382:PHE:CE2	2.53	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:D:357:ASP:OD2	1:D:361:ASN:HB2	2.18	0.44
1:E:189:THR:HG23	1:E:190:PRO:HD2	2.00	0.44
1:E:397:MSE:HE3	3:E:560:HOH:O	2.17	0.44
1:F:439:ARG:O	1:F:443:ILE:HG13	2.18	0.44
1:A:321:LEU:O	1:A:325:LYS:HB2	2.18	0.44
1:B:221:PHE:CE1	1:B:223:PRO:HD3	2.52	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:E:89:LEU:O	1:E:93:ILE:HG13	2.18	0.44
1:F:27:THR:O	1:F:31:ASN:ND2	2.51	0.44
1:B:131:THR:HG22	1:B:133:ASP:H	1.83	0.44
1:F:22:GLY:HA2	1:F:58:PHE:O	2.18	0.44
1:F:92:LEU:CD1	1:F:97:SER:HB2	2.47	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: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: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: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:A:357:ASP:N	3:A:536:HOH:O	2.51	0.43
1:B:27:THR:O	1:B:28:PRO:C	2.56	0.43
1:B:293:LEU:O	1:B:298:ARG:HB3	2.18	0.43
1:E:357:ASP:HA	1:E:406:VAL:O	2.19	0.43
1:F:252:PHE:HB2	1:F:277:PRO:HG2	2.01	0.43
1:B:131:THR:HG21	1:B:133:ASP:OD1	2.17	0.43
1:B:189:THR:HG23	1:B:190:PRO:HD2	2.00	0.43
1:B:257:SER:H	1:B:283:THR:CG2	2.30	0.43
1:C:242:GLU:OE2	1:C:247:ARG:NH2	2.51	0.43
1:C:321:LEU:O	1:C:325:LYS:HB2	2.18	0.43
1:C:356:ALA:O	1:C:405:PHE:HA	2.19	0.43
1:D:256:GLN:CA	1:D:283:THR:HG22	2.46	0.43
1:D:92:LEU:CD1	1:D:97:SER:HB2	2.48	0.43
1:F:331:ARG:CZ	3:F:527:HOH:O	2.66	0.43
1:A:27:THR:O	1:A:28:PRO:C	2.57	0.43
1:A:83:TYR:CZ	1:A:374:ASN:HB3	2.53	0.43
1:C:27:THR:HA	1:C:62:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:145:LEU:HB3	1:A:146:PRO:CD	2.49	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:E:173:LEU:O	1:E:174:CYS:HB3	2.19	0.43
1:F:280:ASN:HD22	1:F:301:PHE:HB3	1.82	0.43
1:C:145:LEU:HB3	1:C:146:PRO:CD	2.49	0.43
1:E:338:ASN:HA	1:E:339:PRO:HD3	1.91	0.43
1:E:356:ALA:O	1:E:405:PHE:HA	2.18	0.43
1:F:138:PRO:HG3	1:F:145:LEU:HD21	2.01	0.43
1:F:63:THR:HB	1:F:67:LEU:HG	2.00	0.43
1:A:89:LEU:O	1:A:93:ILE:HG13	2.19	0.43
1:B:242:GLU:OE2	1:B:247:ARG:NH2	2.51	0.43
1:B:284:GLU:HG3	1:B:382:PHE:CE2	2.53	0.43
1:C:218:GLU:HG3	1:C:219:SER:H	1.84	0.43
1:C:284:GLU:HG3	1:C:382:PHE:CE2	2.54	0.43
1:C:468:THR:HA	1:C:469:PRO:HD3	1.84	0.43
1:F:27:THR:O	1:F:28:PRO:C	2.57	0.43
1:F:361:ASN:C	1:F:362:ILE:HD12	2.38	0.43
1:C:276:ILE:O	1:C:298:ARG:NH1	2.52	0.43
1:C:387:TYR:CE2	1:D:179:PRO:HG2	2.52	0.43
1:C:439:ARG:O	1:C:443:ILE:HG13	2.18	0.43
1:C:444:ILE:HA	1:C:448:VAL:CG2	2.48	0.43
1:E:284:GLU:HG3	1:E:382:PHE:CE2	2.54	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:F:359:PHE:CE2	1:F:469:PRO:HD2	2.53	0.43
1:A:453:ARG:O	1:A:457:ARG:HG3	2.19	0.43
1:C:283:THR:HB	1:C:284:GLU:H	1.68	0.43
1:D:227:VAL:HG11	1:D:394:PRO:HB3	2.01	0.43
1:C:467:GLN:N	1:D:94:ASN:HD22	2.14	0.43
1:E:145:LEU:HB3	1:E:146:PRO:CD	2.49	0.43
1:E:167:ILE:HD13	1:E:167:ILE:HA	1.84	0.43
1:E:227:VAL:HG11	1:E:394:PRO:HB3	2.01	0.43
1:A:356:ALA:O	1:A:405:PHE:HA	2.19	0.42
1:A:403:SER:H	1:A:488:MSE:SE	2.52	0.42
1:B:468:THR:HA	1:B:469:PRO:HD3	1.83	0.42
1:F:397:MSE:HB3	1:F:402:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:409:VAL:HG23	1:F:412:HIS:CD2	2.54	0.42
1:B:92:LEU:CD1	1:B:97:SER:HB2	2.49	0.42
1:C:355:GLU:HG3	1:C:409:VAL:HG12	2.01	0.42
1:D:293:LEU:O	1:D:298:ARG:HB3	2.19	0.42
1:F:184:GLU:O	1:F:186:PRO:HD3	2.19	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: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:B:357:ASP:OD2	1:B:361:ASN:HB2	2.19	0.42
1:B:63:THR:HB	1:B:67:LEU:HG	2.02	0.42
1:D:94:ASN:ND2	1:D:372:MSE:H	2.01	0.42
1:D:22:GLY:HA2	1:D:58:PHE:O	2.20	0.42
1:E:166:GLU:O	1:E:325:LYS:HE2	2.19	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: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:B:487:ASP:HB3	1:B:490:ASN:ND2	2.35	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:293:LEU:HD22	1:D:298:ARG:CG	2.45	0.42
1:D:409:VAL:HG23	1:D:412:HIS:CD2	2.54	0.42
1:F:240:VAL:CG2	3:F:511:HOH:O	2.67	0.42
1:F:468:THR:HA	1:F:469:PRO:HD3	1.82	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:287:GLN:NE2	1:D:290:VAL:HG23	2.35	0.42
1:D:267:LEU:O	1:D:293:LEU:HD11	2.20	0.42
1:D:318:TYR:HA	1:D:321:LEU:HD13	2.01	0.42
1:D:357:ASP:HA	1:D:406:VAL:O	2.20	0.42
1:E:409:VAL:HG23	1:E:412:HIS:CD2	2.54	0.42
1:F:83:TYR:CZ	1:F:374:ASN:HB3	2.54	0.42
1:A:221:PHE:CE1	1:A:223:PRO:HB3	2.54	0.42
1:B:356:ALA:O	1:B:405:PHE:HA	2.20	0.42
1:C:218:GLU:CG	1:C:219:SER:N	2.83	0.42
1:D:354:LEU:HD11	1:D:373:MSE:HG3	2.02	0.42
1:F:236:ALA:O	1:F:240:VAL:HG13	2.19	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:A:236:ALA:O	1:A:240:VAL:HG13	2.19	0.42
1:B:158:GLU:OE1	3:B:513:HOH:O	2.21	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:A:67:LEU:HB3	1:A:68:ASP:H	1.77	0.41
1:B:54:LYS:HG2	1:B:76:ALA:HA	2.01	0.41
1:C:163:HIS:HA	1:C:164:PRO:HD2	1.94	0.41
1:C:357:ASP:HA	1:C:406:VAL:O	2.19	0.41
1:C:435:ASN:ND2	1:C:438:GLU:CG	2.83	0.41
1:E:288:ASP:HB2	3:E:510:HOH:O	2.20	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:167:ILE:HD13	1:D:167:ILE:HA	1.85	0.41
1:D:453:ARG:O	1:D:457:ARG:HG3	2.20	0.41
1:F:280:ASN:ND2	1:F:300:LYS:HB2	2.34	0.41
1:A:221:PHE:CE1	1:A:223:PRO:HD3	2.55	0.41
1:B:22:GLY:HA2	1:B:58:PHE:O	2.20	0.41
1:D:138:PRO:HG3	1:D:145:LEU:HD21	2.00	0.41
1:D:221:PHE:CZ	1:D:223:PRO:HG3	2.55	0.41
1:D:83:TYR:CZ	1:D:374:ASN:HB3	2.56	0.41
1:D:468:THR:HA	1:D:469:PRO:HD3	1.83	0.41
1:E:387:TYR:HD1	1:E:388:VAL:HG23	1.85	0.41
1:F:221:PHE:CZ	1:F:223:PRO:HG3	2.56	0.41
1:F:357:ASP:HA	1:F:406:VAL:O	2.19	0.41
1:A:163:HIS:HA	1:A:164:PRO:HD2	1.92	0.41
1:A:221:PHE:CZ	1:A:223:PRO:HG3	2.55	0.41
1:B:136:ILE:HD12	1:B:136:ILE:N	2.35	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:D:163:HIS:HA	1:D:164:PRO:HD2	1.95	0.41
1:E:184:GLU:O	1:E:186:PRO:HD3	2.20	0.41
1:E:83:TYR:CZ	1:E:374:ASN:HB3	2.55	0.41
1:F:131:THR:HG22	1:F:133:ASP:H	1.85	0.41
1:F:17:HIS:CD2	1:F:53:PHE:HA	2.55	0.41
1:F:63:THR:OG1	1:F:67:LEU:HB3	2.20	0.41
1:A:355:GLU:HG3	1:A:409:VAL:HG12	2.02	0.41
1:B:341:ILE:HD13	1:B:341:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:PHE:O	1:C:27:THR:HG23	2.21	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:F:54:LYS:HG2	1:F:76:ALA:HA	2.01	0.41
1:B:138:PRO:HG3	1:B:145:LEU:HD21	2.02	0.41
1:B:145:LEU:HB3	1:B:146:PRO:CD	2.51	0.41
1:B:184:GLU:O	1:B:186:PRO:HD3	2.21	0.41
1:B:354:LEU:HD11	1:B:373:MSE:HG3	2.03	0.41
1:B:227:VAL:HG11	1:B:394:PRO:HB3	2.03	0.41
1:E:293:LEU:O	1:E:298:ARG:HB3	2.20	0.41
1:A:221:PHE:CD1	1:A:223:PRO:HD3	2.56	0.41
1:B:221:PHE:CD1	1:B:223:PRO:HD3	2.56	0.41
1:C:26:PHE:C	1:C:27:THR:HG23	2.40	0.41
1:D:221:PHE:CD1	1:D:223:PRO:HD3	2.56	0.41
1:D:252:PHE:HB2	1:D:277:PRO:HG2	2.02	0.41
1:D:356:ALA:O	1:D:405:PHE:HA	2.20	0.41
1:F:131:THR:HG21	1:F:133:ASP:OD1	2.21	0.41
1:F:356:ALA:O	1:F:405:PHE:HA	2.20	0.41
1:F:407:PRO:HD2	3:F:538:HOH:O	2.20	0.41
1:D:131:THR:HG22	1:D:133:ASP:H	1.86	0.41
1:E:127:VAL:HG12	1:E:128:ALA:N	2.36	0.41
1:E:252:PHE:O	1:E:253:LEU:HD13	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: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:D:252:PHE:O	1:D:253:LEU:HD13	2.21	0.41
1:F:136:ILE:HD12	1:F:136:ILE:N	2.35	0.41
1:F:26:PHE:O	1:F:27:THR:HG23	2.21	0.41
1:D:102:ASP:N	1:D:102:ASP:OD2	2.51	0.41
1:E:256:GLN:CA	1:E:283:THR:HG22	2.45	0.41
1:F:167:ILE:HA	1:F:167:ILE:HD13	1.84	0.41
1:A:218:GLU:HG3	1:A:219:SER:H	1.85	0.40
1:A:284:GLU:HG3	1:A:382:PHE:HE2	1.86	0.40
1:B:221:PHE:CZ	1:B:223:PRO:HG3	2.56	0.40
1:C:147:THR:HG22	1:C:151:LEU:HD22	2.03	0.40
1:D:145:LEU:HB3	1:D:146:PRO:CD	2.51	0.40
1:E:163:HIS:HA	1:E:164:PRO:HD2	1.93	0.40
1:E:22:GLY:HA2	1:E:58:PHE:O	2.21	0.40
1:E:468:THR:HA	1:E:469:PRO:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PRO:HG3	1:A:145:LEU:HD21	2.02	0.40
1:A:267:LEU:O	1:A:293:LEU:HD11	2.21	0.40
1:A:409:VAL:HG23	1:A:412:HIS:CD2	2.57	0.40
1:B:26:PHE:CE1	1:B:61:ALA:HB2	2.55	0.40
1:B:409:VAL:HG23	1:B:412:HIS:CD2	2.56	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: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:E:439:ARG:O	1:E:443:ILE:HG13	2.21	0.40
1:F:283:THR:HB	1:F:284:GLU:H	1.69	0.40
1:A:124:ILE:CD1	1:A:156:ILE:HD12	2.51	0.40
1:A:189:THR:HG23	1:A:190:PRO:HD2	2.04	0.40
1:B:403:SER:H	1:B:488:MSE:SE	2.55	0.40
1:C:294:MSE:CE	1:C:324:PHE:CD2	3.04	0.40
1:E:54:LYS:HG2	1:E:76:ALA:HA	2.02	0.40
1:F:35:VAL:O	1:F:39:ILE:HG12	2.22	0.40
1:A:131:THR:HG22	1:A:133:ASP:H	1.85	0.40
1:A:22:GLY:HA2	1:A:58:PHE:O	2.21	0.40
1:A:26:PHE:C	1:A:27:THR:HG23	2.42	0.40
1:C:284:GLU:HG3	1:C:382:PHE:HE2	1.85	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:E:92:LEU:HB2	3:E:539:HOH:O	2.20	0.40
1:F:267:LEU:O	1:F:293:LEU:HD11	2.21	0.40
1:F:378:GLY:O	1:F:382:PHE:HD2	2.04	0.40
1:F:453:ARG:CD	3:F:515:HOH:O	2.69	0.40
1:B:124:ILE:CD1	1:B:156:ILE:HD12	2.51	0.40
1:B:357:ASP:HA	1:B:406:VAL:O	2.21	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:E:131:THR:HG21	1:E:133:ASP:OD1	2.22	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%)	25	50	
1	B	494/506 (98%)	462 (94%)	29 (6%)	3 (1%)	25	50	
1	C	494/506 (98%)	460 (93%)	31 (6%)	3 (1%)	25	50	
1	D	494/506 (98%)	461 (93%)	29 (6%)	4 (1%)	19	43	
1	E	494/506 (98%)	461 (93%)	29 (6%)	4 (1%)	19	43	
1	F	494/506 (98%)	460 (93%)	30 (6%)	4 (1%)	19	43	
All	All	2964/3036 (98%)	2762 (93%)	181 (6%)	21 (1%)	22	46	

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%)	29	57
1	B	416/413 (101%)	398 (96%)	18 (4%)	29	57
1	C	416/413 (101%)	397 (95%)	19 (5%)	27	54
1	D	416/413 (101%)	397 (95%)	19 (5%)	27	54
1	E	416/413 (101%)	398 (96%)	18 (4%)	29	57
1	F	416/413 (101%)	398 (96%)	18 (4%)	29	57
All	All	2496/2478 (101%)	2386 (96%)	110 (4%)	28	56

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%)	1.75	159 (32%) 0 0	6, 7, 18, 30	0
1	B	484/506 (95%)	1.82	184 (38%) 0 0	6, 7, 18, 30	0
1	C	484/506 (95%)	1.75	170 (35%) 0 0	6, 7, 18, 30	0
1	D	484/506 (95%)	1.91	191 (39%) 0 0	6, 7, 18, 30	0
1	E	484/506 (95%)	2.58	310 (64%) 0 0	6, 7, 18, 30	0
1	F	484/506 (95%)	2.62	307 (63%) 0 0	6, 7, 18, 30	0
All	All	2904/3036 (95%)	2.07	1321 (45%) 0 0	6, 7, 18, 30	0

All (1321) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	427	GLY	8.4
1	F	134	GLY	7.5
1	F	232	GLY	7.2
1	C	85	SER	6.9
1	F	299	ILE	6.8
1	F	227	VAL	6.8
1	E	405	PHE	6.6
1	E	393	THR	6.6
1	E	365	THR	6.5
1	F	99	SER	6.3
1	F	127	VAL	6.3
1	E	483	ALA	6.3
1	F	290	VAL	6.3
1	E	345	LEU	6.3
1	E	383	THR	6.2
1	F	149	CYS	6.2
1	E	60	GLY	6.1
1	D	207	VAL	6.0
1	E	326	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	E	318	TYR	5.9
1	F	199	VAL	5.9
1	F	449	HIS	5.9
1	A	222	ALA	5.9
1	F	407	PRO	5.8
1	E	116	PHE	5.8
1	F	58	PHE	5.8
1	F	208	GLY	5.8
1	F	136	ILE	5.7
1	F	229	GLN	5.7
1	E	222	ALA	5.6
1	F	478	PHE	5.6
1	E	157	VAL	5.6
1	D	55	ILE	5.5
1	F	138	PRO	5.4
1	E	125	ILE	5.4
1	E	447	CYS	5.4
1	D	220	ASP	5.4
1	E	85	SER	5.4
1	C	219	SER	5.4
1	E	33	LYS	5.4
1	A	221	PHE	5.4
1	B	122	VAL	5.3
1	F	270	LEU	5.3
1	F	376	ILE	5.3
1	F	130	VAL	5.3
1	E	352	THR	5.3
1	F	328	ILE	5.3
1	F	190	PRO	5.3
1	F	350	ILE	5.3
1	D	410	ALA	5.2
1	E	203	PRO	5.2
1	F	201	VAL	5.2
1	D	116	PHE	5.1
1	E	370	THR	5.1
1	A	125	ILE	5.1
1	F	318	TYR	5.1
1	F	382	PHE	5.1
1	D	63	THR	5.1
1	E	477	ALA	5.1
1	F	467	GLN	5.1
1	D	221	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	217	ASP	5.1
1	F	462	LEU	5.1
1	E	363	ASN	5.1
1	D	307	LEU	5.0
1	D	118	GLY	5.0
1	F	223	PRO	5.0
1	F	221	PHE	5.0
1	E	89	LEU	5.0
1	E	223	PRO	5.0
1	F	494	GLU	5.0
1	D	354	LEU	5.0
1	F	496	TYR	4.9
1	F	361	ASN	4.9
1	F	123	ALA	4.9
1	C	350	ILE	4.9
1	F	248	ILE	4.9
1	F	291	ILE	4.9
1	F	447	CYS	4.9
1	E	376	ILE	4.9
1	F	11	ALA	4.9
1	D	352	THR	4.9
1	D	137	LEU	4.8
1	D	241	SER	4.8
1	E	432	ARG	4.8
1	F	289	ALA	4.8
1	A	398	LYS	4.8
1	F	359	PHE	4.8
1	F	286	ILE	4.8
1	F	274	PRO	4.8
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	D	315	GLN	4.8
1	E	410	ALA	4.7
1	F	374	ASN	4.7
1	E	52	PRO	4.7
1	F	282	TYR	4.7
1	E	322	ASP	4.7
1	F	72	ALA	4.6
1	F	409	VAL	4.6
1	F	124	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	383	THR	4.6
1	B	2	ALA	4.6
1	F	230	ALA	4.6
1	B	255	LEU	4.6
1	E	119	LYS	4.6
1	F	257	SER	4.6
1	F	472	LEU	4.6
1	E	259	VAL	4.6
1	F	148	ILE	4.6
1	C	496	TYR	4.6
1	E	353	ALA	4.6
1	F	276	ILE	4.5
1	E	159	LEU	4.5
1	F	263	ALA	4.5
1	E	81	THR	4.5
1	F	185	LEU	4.5
1	A	21	VAL	4.5
1	E	388	VAL	4.5
1	E	428	VAL	4.5
1	B	231	ILE	4.5
1	E	328	ILE	4.5
1	E	307	LEU	4.5
1	E	209	VAL	4.5
1	D	285	VAL	4.5
1	F	85	SER	4.5
1	B	112	LEU	4.5
1	B	221	PHE	4.4
1	B	400	GLY	4.4
1	E	77	VAL	4.4
1	E	464	VAL	4.4
1	B	99	SER	4.4
1	C	374	ASN	4.4
1	F	209	VAL	4.4
1	F	117	TYR	4.4
1	F	68	ASP	4.4
1	F	193	ARG	4.4
1	A	34	VAL	4.4
1	F	491	VAL	4.4
1	B	43	ALA	4.4
1	F	426	TRP	4.4
1	E	224	LEU	4.4
1	E	204	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	449	HIS	4.3
1	F	50	GLY	4.3
1	B	370	THR	4.3
1	F	325	LYS	4.3
1	F	323	PHE	4.3
1	A	186	PRO	4.3
1	A	40	ALA	4.3
1	E	2	ALA	4.3
1	F	238	PHE	4.3
1	D	318	TYR	4.3
1	E	354	LEU	4.2
1	C	63	THR	4.2
1	F	207	VAL	4.2
1	F	188	TYR	4.2
1	E	185	LEU	4.2
1	E	102	ASP	4.2
1	F	8	ALA	4.2
1	E	21	VAL	4.2
1	E	309	VAL	4.2
1	A	477	ALA	4.2
1	E	422	ILE	4.2
1	E	14	PHE	4.2
1	D	32	PRO	4.2
1	D	112	LEU	4.2
1	A	117	TYR	4.1
1	B	452	TYR	4.1
1	E	492	ARG	4.1
1	D	136	ILE	4.1
1	F	59	THR	4.1
1	C	93	ILE	4.1
1	D	167	ILE	4.1
1	E	151	LEU	4.1
1	F	194	ILE	4.1
1	D	147	THR	4.1
1	F	269	ALA	4.1
1	B	7	THR	4.1
1	F	326	ASP	4.1
1	E	469	PRO	4.1
1	D	327	LYS	4.1
1	E	360	GLY	4.1
1	E	12	ALA	4.1
1	D	365	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	173	LEU	4.1
1	F	112	LEU	4.1
1	F	327	LYS	4.1
1	E	42	ARG	4.0
1	A	2	ALA	4.0
1	F	264	ASN	4.0
1	C	32	PRO	4.0
1	E	349	THR	4.0
1	C	352	THR	4.0
1	F	330	LEU	4.0
1	E	24	SER	4.0
1	E	418	SER	4.0
1	F	77	VAL	4.0
1	F	228	THR	4.0
1	D	21	VAL	4.0
1	E	319	ALA	4.0
1	E	337	ASN	4.0
1	F	329	LEU	4.0
1	C	99	SER	4.0
1	F	351	ASN	4.0
1	E	178	ASP	4.0
1	D	491	VAL	4.0
1	F	63	THR	3.9
1	D	156	ILE	3.9
1	B	8	ALA	3.9
1	E	240	VAL	3.9
1	D	393	THR	3.9
1	E	379	SER	3.9
1	E	98	THR	3.9
1	E	415	SER	3.9
1	E	296	LYS	3.9
1	A	339	PRO	3.9
1	E	144	ILE	3.9
1	B	326	ASP	3.9
1	B	58	PHE	3.9
1	F	410	ALA	3.9
1	D	350	ILE	3.9
1	A	99	SER	3.9
1	E	173	LEU	3.9
1	A	7	THR	3.9
1	E	188	TYR	3.9
1	E	118	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	388	VAL	3.9
1	E	389	SER	3.9
1	A	369	GLY	3.9
1	F	30	GLY	3.9
1	E	278	ALA	3.8
1	E	423	ILE	3.8
1	F	300	LYS	3.8
1	B	3	LEU	3.8
1	E	75	ASP	3.8
1	E	340	GLU	3.8
1	F	122	VAL	3.8
1	C	349	THR	3.8
1	F	475	CYS	3.8
1	F	284	GLU	3.8
1	D	37	ALA	3.8
1	D	146	PRO	3.8
1	D	18	ASN	3.8
1	F	402	ILE	3.8
1	E	108	LEU	3.8
1	A	64	GLY	3.8
1	E	228	THR	3.8
1	B	286	ILE	3.8
1	E	286	ILE	3.8
1	B	448	VAL	3.8
1	D	322	ASP	3.8
1	D	349	THR	3.8
1	F	107	THR	3.8
1	E	26	PHE	3.8
1	E	411	HIS	3.8
1	B	342	VAL	3.8
1	E	218	GLU	3.8
1	F	187	VAL	3.8
1	F	161	ASP	3.8
1	E	66	ARG	3.7
1	A	120	VAL	3.7
1	A	67	LEU	3.7
1	A	455	LEU	3.7
1	E	93	ILE	3.7
1	F	44	ILE	3.7
1	E	143	GLY	3.7
1	E	17	HIS	3.7
1	E	61	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	350	ILE	3.7
1	F	213	SER	3.7
1	E	6	ILE	3.7
1	D	431	LEU	3.7
1	C	28	PRO	3.7
1	E	27	THR	3.7
1	E	212	THR	3.7
1	E	142	VAL	3.7
1	B	64	GLY	3.7
1	B	339	PRO	3.7
1	F	147	THR	3.7
1	F	41	LYS	3.7
1	D	26	PHE	3.7
1	E	51	ASN	3.7
1	F	128	ALA	3.7
1	E	156	ILE	3.7
1	C	403	SER	3.7
1	E	361	ASN	3.6
1	F	370	THR	3.6
1	E	79	PHE	3.6
1	E	255	LEU	3.6
1	E	95	ASN	3.6
1	F	412	HIS	3.6
1	A	122	VAL	3.6
1	C	136	ILE	3.6
1	E	199	VAL	3.6
1	F	155	ILE	3.6
1	A	131	THR	3.6
1	F	36	PRO	3.6
1	A	187	VAL	3.6
1	A	197	PRO	3.6
1	D	383	THR	3.6
1	E	92	LEU	3.6
1	A	443	ILE	3.6
1	A	452	TYR	3.6
1	F	252	PHE	3.6
1	C	360	GLY	3.6
1	D	77	VAL	3.6
1	E	53	PHE	3.6
1	F	167	ILE	3.6
1	F	46	ALA	3.6
1	F	83	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	36	PRO	3.5
1	D	317	ILE	3.5
1	F	283	THR	3.5
1	E	49	LYS	3.5
1	F	389	SER	3.5
1	D	239	LEU	3.5
1	C	133	ASP	3.5
1	A	195	GLY	3.5
1	E	15	VAL	3.5
1	E	375	GLY	3.5
1	F	464	VAL	3.5
1	E	31	ASN	3.5
1	E	216	ASN	3.5
1	C	239	LEU	3.5
1	F	321	LEU	3.5
1	E	335	TYR	3.5
1	F	26	PHE	3.5
1	B	218	GLU	3.5
1	F	179	PRO	3.5
1	D	300	LYS	3.5
1	C	223	PRO	3.5
1	E	189	THR	3.5
1	F	224	LEU	3.5
1	D	102	ASP	3.5
1	A	89	LEU	3.5
1	E	248	ILE	3.5
1	F	200	GLN	3.5
1	B	305	CYS	3.4
1	E	16	HIS	3.4
1	E	306	SER	3.4
1	B	186	PRO	3.4
1	D	164	PRO	3.4
1	E	28	PRO	3.4
1	E	164	PRO	3.4
1	C	156	ILE	3.4
1	E	414	HIS	3.4
1	D	97	SER	3.4
1	E	310	SER	3.4
1	E	120	VAL	3.4
1	E	105	LEU	3.4
1	D	266	VAL	3.4
1	F	417	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	398	LYS	3.4
1	E	37	ALA	3.4
1	E	438	GLU	3.4
1	F	452	TYR	3.4
1	E	436	PRO	3.4
1	E	402	ILE	3.4
1	F	56	GLY	3.4
1	B	419	VAL	3.4
1	F	346	GLY	3.4
1	F	47	HIS	3.4
1	F	18	ASN	3.4
1	E	295	LYS	3.4
1	B	210	VAL	3.4
1	D	208	GLY	3.4
1	E	232	GLY	3.4
1	C	41	LYS	3.4
1	C	166	GLU	3.4
1	C	348	ILE	3.3
1	D	403	SER	3.3
1	F	163	HIS	3.3
1	D	135	LYS	3.3
1	C	31	ASN	3.3
1	A	108	LEU	3.3
1	E	20	ASN	3.3
1	F	334	GLU	3.3
1	D	375	GLY	3.3
1	D	262	VAL	3.3
1	B	447	CYS	3.3
1	E	245	ALA	3.3
1	F	25	GLY	3.3
1	B	394	PRO	3.3
1	F	133	ASP	3.3
1	D	171	HIS	3.3
1	F	324	PHE	3.3
1	D	4	ARG	3.3
1	B	223	PRO	3.3
1	C	225	ASP	3.3
1	C	10	GLU	3.3
1	E	491	VAL	3.3
1	A	234	ASN	3.3
1	F	476	PHE	3.3
1	F	429	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	224	LEU	3.3
1	B	224	LEU	3.3
1	F	105	LEU	3.3
1	E	150	ARG	3.3
1	F	237	ALA	3.3
1	C	447	CYS	3.3
1	D	274	PRO	3.3
1	E	131	THR	3.3
1	F	285	VAL	3.3
1	D	68	ASP	3.3
1	D	219	SER	3.2
1	C	259	VAL	3.2
1	D	227	VAL	3.2
1	E	266	VAL	3.2
1	F	231	ILE	3.2
1	E	192	ASP	3.2
1	B	264	ASN	3.2
1	B	167	ILE	3.2
1	D	44	ILE	3.2
1	F	390	ILE	3.2
1	D	177	LEU	3.2
1	E	117	TYR	3.2
1	B	74	ALA	3.2
1	B	70	VAL	3.2
1	B	130	VAL	3.2
1	C	402	ILE	3.2
1	E	183	ARG	3.2
1	B	165	LYS	3.2
1	D	230	ALA	3.2
1	E	48	GLU	3.2
1	E	448	VAL	3.2
1	F	93	ILE	3.2
1	A	190	PRO	3.2
1	B	336	SER	3.2
1	F	256	GLN	3.2
1	A	448	VAL	3.2
1	D	70	VAL	3.2
1	F	142	VAL	3.2
1	A	217	ASP	3.2
1	B	265	ALA	3.2
1	E	138	PRO	3.2
1	E	462	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	127	VAL	3.2
1	D	202	ASP	3.2
1	F	319	ALA	3.2
1	A	364	SER	3.2
1	B	465	LYS	3.2
1	C	379	SER	3.2
1	E	377	GLY	3.2
1	F	219	SER	3.2
1	F	430	ASP	3.1
1	B	113	ARG	3.1
1	F	226	PRO	3.1
1	B	139	THR	3.1
1	E	280	ASN	3.1
1	E	314	ILE	3.1
1	F	29	ALA	3.1
1	A	460	LEU	3.1
1	F	490	ASN	3.1
1	F	340	GLU	3.1
1	E	104	HIS	3.1
1	E	426	TRP	3.1
1	D	342	VAL	3.1
1	D	299	ILE	3.1
1	F	55	ILE	3.1
1	F	320	ASN	3.1
1	E	272	ASP	3.1
1	E	3	LEU	3.1
1	E	76	ALA	3.1
1	E	341	ILE	3.1
1	F	398	LYS	3.1
1	A	102	ASP	3.1
1	A	349	THR	3.1
1	B	369	GLY	3.1
1	F	169	GLY	3.1
1	B	269	ALA	3.1
1	B	429	ALA	3.1
1	D	353	ALA	3.1
1	A	436	PRO	3.1
1	E	317	ILE	3.1
1	F	341	ILE	3.1
1	B	427	GLY	3.1
1	C	77	VAL	3.1
1	C	409	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	351	ASN	3.1
1	F	137	LEU	3.1
1	B	402	ILE	3.1
1	E	190	PRO	3.1
1	F	444	ILE	3.1
1	E	496	TYR	3.1
1	D	389	SER	3.1
1	E	112	LEU	3.1
1	E	263	ALA	3.1
1	F	303	SER	3.1
1	F	345	LEU	3.1
1	A	182	ARG	3.1
1	D	348	ILE	3.1
1	F	297	GLY	3.0
1	F	414	HIS	3.0
1	B	131	THR	3.0
1	C	26	PHE	3.0
1	F	262	VAL	3.0
1	A	255	LEU	3.0
1	E	149	CYS	3.0
1	D	283	THR	3.0
1	E	34	VAL	3.0
1	C	265	ALA	3.0
1	C	289	ALA	3.0
1	D	92	LEU	3.0
1	D	108	LEU	3.0
1	E	308	SER	3.0
1	E	11	ALA	3.0
1	F	239	LEU	3.0
1	B	258	GLY	3.0
1	D	169	GLY	3.0
1	A	79	PHE	3.0
1	C	324	PHE	3.0
1	F	54	LYS	3.0
1	F	70	VAL	3.0
1	F	118	GLY	3.0
1	F	258	GLY	3.0
1	F	5	PHE	3.0
1	F	211	ARG	3.0
1	D	81	THR	3.0
1	F	153	ASP	3.0
1	E	270	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	292	ALA	3.0
1	F	162	LYS	3.0
1	F	387	TYR	3.0
1	B	21	VAL	3.0
1	B	462	LEU	3.0
1	E	45	ALA	3.0
1	F	298	ARG	3.0
1	E	478	PHE	3.0
1	F	116	PHE	3.0
1	F	34	VAL	3.0
1	F	456	LEU	3.0
1	F	343	ARG	3.0
1	E	480	GLN	3.0
1	B	471	ASN	3.0
1	F	385	ASN	3.0
1	B	87	LYS	3.0
1	B	227	VAL	3.0
1	F	159	LEU	3.0
1	B	195	GLY	3.0
1	F	466	GLY	3.0
1	C	237	ALA	3.0
1	B	146	PRO	3.0
1	C	277	PRO	3.0
1	C	206	ILE	2.9
1	B	101	PHE	2.9
1	B	424	SER	2.9
1	A	103	LEU	2.9
1	D	134	GLY	2.9
1	E	482	LEU	2.9
1	D	144	ILE	2.9
1	F	6	ILE	2.9
1	A	324	PHE	2.9
1	B	241	SER	2.9
1	D	306	SER	2.9
1	C	60	GLY	2.9
1	E	139	THR	2.9
1	E	177	LEU	2.9
1	F	108	LEU	2.9
1	B	347	VAL	2.9
1	B	367	VAL	2.9
1	D	130	VAL	2.9
1	D	199	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	197	PRO	2.9
1	A	358	ILE	2.9
1	B	358	ILE	2.9
1	C	18	ASN	2.9
1	D	376	ILE	2.9
1	F	24	SER	2.9
1	B	377	GLY	2.9
1	C	208	GLY	2.9
1	A	370	THR	2.9
1	C	482	LEU	2.9
1	B	332	PRO	2.9
1	E	176	PRO	2.9
1	A	357	ASP	2.9
1	D	216	ASN	2.9
1	F	218	GLU	2.9
1	C	299	ILE	2.9
1	A	23	PHE	2.9
1	C	116	PHE	2.9
1	D	42	ARG	2.9
1	C	177	LEU	2.9
1	E	59	THR	2.9
1	A	207	VAL	2.9
1	E	83	TYR	2.9
1	F	21	VAL	2.9
1	A	36	PRO	2.9
1	A	91	ASN	2.9
1	E	291	ILE	2.9
1	D	462	LEU	2.9
1	C	413	ASP	2.9
1	F	413	ASP	2.9
1	B	155	ILE	2.9
1	E	55	ILE	2.9
1	B	81	THR	2.9
1	D	117	TYR	2.9
1	E	146	PRO	2.9
1	E	371	ARG	2.9
1	F	277	PRO	2.9
1	E	25	GLY	2.9
1	D	303	SER	2.9
1	E	106	SER	2.9
1	E	219	SER	2.9
1	E	348	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	98	THR	2.9
1	F	140	THR	2.9
1	F	468	THR	2.9
1	F	369	GLY	2.8
1	E	241	SER	2.8
1	E	300	LYS	2.8
1	D	59	THR	2.8
1	F	217	ASP	2.8
1	B	40	ALA	2.8
1	C	315	GLN	2.8
1	E	367	VAL	2.8
1	C	378	GLY	2.8
1	E	167	ILE	2.8
1	F	53	PHE	2.8
1	A	293	LEU	2.8
1	B	239	LEU	2.8
1	C	370	THR	2.8
1	E	172	ASP	2.8
1	A	227	VAL	2.8
1	A	356	ALA	2.8
1	E	130	VAL	2.8
1	E	165	LYS	2.8
1	F	347	VAL	2.8
1	E	475	CYS	2.8
1	B	6	ILE	2.8
1	B	182	ARG	2.8
1	E	147	THR	2.8
1	F	401	LYS	2.8
1	D	436	PRO	2.8
1	E	271	GLY	2.8
1	F	106	SER	2.8
1	B	317	ILE	2.8
1	F	301	PHE	2.8
1	E	330	LEU	2.8
1	F	129	ASP	2.8
1	B	29	ALA	2.8
1	F	157	VAL	2.8
1	E	403	SER	2.8
1	C	256	GLN	2.8
1	D	362	ILE	2.8
1	D	460	LEU	2.8
1	E	251	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	476	PHE	2.8
1	F	177	LEU	2.8
1	F	233	ASP	2.8
1	B	352	THR	2.8
1	A	262	VAL	2.8
1	A	219	SER	2.8
1	C	306	SER	2.8
1	A	58	PHE	2.8
1	A	167	ILE	2.8
1	B	354	LEU	2.8
1	E	444	ILE	2.8
1	B	107	THR	2.8
1	F	392	THR	2.8
1	E	193	ARG	2.8
1	E	244	LYS	2.8
1	C	309	VAL	2.8
1	C	467	GLN	2.8
1	A	326	ASP	2.8
1	C	79	PHE	2.8
1	C	471	ASN	2.8
1	B	474	CYS	2.8
1	E	82	PRO	2.7
1	E	282	TYR	2.7
1	A	427	GLY	2.7
1	E	145	LEU	2.7
1	E	320	ASN	2.7
1	B	461	GLU	2.7
1	D	364	SER	2.7
1	C	83	TYR	2.7
1	C	258	GLY	2.7
1	E	378	GLY	2.7
1	F	126	GLU	2.7
1	F	461	GLU	2.7
1	F	333	GLN	2.7
1	A	465	LYS	2.7
1	D	432	ARG	2.7
1	C	335	TYR	2.7
1	B	189	THR	2.7
1	C	140	THR	2.7
1	F	434	LYS	2.7
1	B	230	ALA	2.7
1	C	45	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	412	HIS	2.7
1	B	184	GLU	2.7
1	B	173	LEU	2.7
1	D	325	LYS	2.7
1	C	147	THR	2.7
1	F	176	PRO	2.7
1	F	35	VAL	2.7
1	F	121	ASP	2.7
1	C	17	HIS	2.7
1	E	479	HIS	2.7
1	C	108	LEU	2.7
1	C	250	LYS	2.7
1	C	478	PHE	2.7
1	F	244	LYS	2.7
1	A	144	ILE	2.7
1	B	274	PRO	2.7
1	C	430	ASP	2.7
1	D	381	ASP	2.7
1	A	235	VAL	2.7
1	C	342	VAL	2.7
1	F	73	GLN	2.7
1	B	108	LEU	2.7
1	B	100	TYR	2.7
1	D	83	TYR	2.7
1	A	82	PRO	2.7
1	B	76	ALA	2.7
1	C	230	ALA	2.7
1	D	165	LYS	2.7
1	F	196	LYS	2.7
1	C	285	VAL	2.7
1	A	291	ILE	2.7
1	C	167	ILE	2.7
1	F	125	ILE	2.7
1	F	154	ARG	2.7
1	C	303	SER	2.7
1	A	274	PRO	2.6
1	B	450	PRO	2.6
1	D	222	ALA	2.6
1	E	180	PRO	2.6
1	B	235	VAL	2.6
1	F	293	LEU	2.6
1	C	248	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	124	ILE	2.6
1	D	341	ILE	2.6
1	B	392	THR	2.6
1	D	368	SER	2.6
1	E	44	ILE	2.6
1	C	64	GLY	2.6
1	F	64	GLY	2.6
1	E	171	HIS	2.6
1	E	313	VAL	2.6
1	F	120	VAL	2.6
1	F	160	ASN	2.6
1	B	460	LEU	2.6
1	C	185	LEU	2.6
1	C	431	LEU	2.6
1	E	137	LEU	2.6
1	C	220	ASP	2.6
1	A	136	ILE	2.6
1	B	248	ILE	2.6
1	D	232	GLY	2.6
1	A	471	ASN	2.6
1	B	309	VAL	2.6
1	D	31	ASN	2.6
1	E	338	ASN	2.6
1	E	406	VAL	2.6
1	F	51	ASN	2.6
1	C	330	LEU	2.6
1	B	217	ASP	2.6
1	D	387	TYR	2.6
1	E	358	ILE	2.6
1	B	152	ALA	2.6
1	B	174	CYS	2.6
1	A	342	VAL	2.6
1	F	419	VAL	2.6
1	C	73	GLN	2.6
1	F	315	GLN	2.6
1	A	218	GLU	2.6
1	B	325	LYS	2.6
1	E	369	GLY	2.6
1	F	312	SER	2.6
1	A	231	ILE	2.6
1	C	6	ILE	2.6
1	D	340	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	39	ILE	2.6
1	E	459	TYR	2.6
1	E	40	ALA	2.6
1	F	450	PRO	2.6
1	C	234	ASN	2.6
1	F	31	ASN	2.6
1	F	344	ARG	2.6
1	B	262	VAL	2.6
1	B	270	LEU	2.6
1	B	23	PHE	2.6
1	D	323	PHE	2.6
1	C	117	TYR	2.6
1	E	254	PRO	2.6
1	C	201	VAL	2.6
1	E	285	VAL	2.6
1	D	158	GLU	2.6
1	F	391	PHE	2.6
1	B	148	ILE	2.6
1	F	180	PRO	2.6
1	A	265	ALA	2.6
1	D	412	HIS	2.6
1	C	187	VAL	2.6
1	B	456	LEU	2.6
1	D	192	ASP	2.6
1	A	101	PHE	2.6
1	B	297	GLY	2.6
1	D	56	GLY	2.6
1	E	279	PHE	2.6
1	C	155	ILE	2.5
1	C	341	ILE	2.5
1	D	273	ASN	2.5
1	C	366	HIS	2.5
1	F	236	ALA	2.5
1	F	487	ASP	2.5
1	D	379	SER	2.5
1	E	234	ASN	2.5
1	F	20	ASN	2.5
1	F	186	PRO	2.5
1	D	483	ALA	2.5
1	A	251	ASP	2.5
1	B	117	TYR	2.5
1	A	112	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	208	GLY	2.5
1	F	48	GLU	2.5
1	D	479	HIS	2.5
1	E	39	ILE	2.5
1	A	484	LYS	2.5
1	B	89	LEU	2.5
1	B	201	VAL	2.5
1	D	145	LEU	2.5
1	E	187	VAL	2.5
1	E	250	LYS	2.5
1	E	431	LEU	2.5
1	F	135	LYS	2.5
1	F	484	LYS	2.5
1	B	324	PHE	2.5
1	F	368	SER	2.5
1	D	218	GLU	2.5
1	B	435	ASN	2.5
1	C	394	PRO	2.5
1	C	125	ILE	2.5
1	E	220	ASP	2.5
1	E	381	ASP	2.5
1	E	451	ASP	2.5
1	C	171	HIS	2.5
1	C	375	GLY	2.5
1	A	282	TYR	2.5
1	D	71	LEU	2.5
1	F	91	ASN	2.5
1	B	371	ARG	2.5
1	A	156	ILE	2.5
1	D	45	ALA	2.5
1	E	155	ILE	2.5
1	A	84	GLN	2.5
1	A	267	LEU	2.5
1	A	201	VAL	2.5
1	B	240	VAL	2.5
1	B	320	ASN	2.5
1	E	325	LYS	2.5
1	A	61	ALA	2.5
1	A	383	THR	2.5
1	C	134	GLY	2.5
1	C	383	THR	2.5
1	A	422	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	423	ILE	2.5
1	B	291	ILE	2.5
1	B	362	ILE	2.5
1	D	104	HIS	2.5
1	E	366	HIS	2.5
1	E	433	GLY	2.5
1	F	365	THR	2.5
1	A	301	PHE	2.5
1	C	327	LYS	2.5
1	F	198	TYR	2.5
1	C	42	ARG	2.5
1	D	197	PRO	2.5
1	B	422	ILE	2.5
1	D	402	ILE	2.5
1	E	440	ALA	2.5
1	F	222	ALA	2.5
1	D	89	LEU	2.5
1	D	240	VAL	2.5
1	E	396	VAL	2.5
1	F	191	SER	2.5
1	D	405	PHE	2.5
1	E	4	ARG	2.5
1	E	86	ASN	2.5
1	A	180	PRO	2.4
1	D	2	ALA	2.4
1	F	109	ALA	2.4
1	D	155	ILE	2.4
1	B	285	VAL	2.4
1	C	301	PHE	2.4
1	D	331	ARG	2.4
1	A	233	ASP	2.4
1	C	361	ASN	2.4
1	E	284	GLU	2.4
1	C	143	GLY	2.4
1	C	484	LYS	2.4
1	E	87	LYS	2.4
1	F	287	GLN	2.4
1	F	43	ALA	2.4
1	F	349	THR	2.4
1	B	137	LEU	2.4
1	B	185	LEU	2.4
1	F	431	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	193	ARG	2.4
1	A	388	VAL	2.4
1	C	493	TRP	2.4
1	F	113	ARG	2.4
1	F	342	VAL	2.4
1	F	415	SER	2.4
1	B	220	ASP	2.4
1	A	165	LYS	2.4
1	C	179	PRO	2.4
1	E	417	HIS	2.4
1	F	164	PRO	2.4
1	B	390	ILE	2.4
1	C	472	LEU	2.4
1	E	390	ILE	2.4
1	A	320	ASN	2.4
1	B	338	ASN	2.4
1	C	68	ASP	2.4
1	D	309	VAL	2.4
1	F	87	LYS	2.4
1	E	315	GLN	2.4
1	C	463	GLY	2.4
1	A	475	CYS	2.4
1	F	82	PRO	2.4
1	C	128	ALA	2.4
1	D	423	ILE	2.4
1	A	20	ASN	2.4
1	A	467	GLN	2.4
1	B	288	ASP	2.4
1	F	220	ASP	2.4
1	F	470	GLN	2.4
1	B	271	GLY	2.4
1	C	466	GLY	2.4
1	D	60	GLY	2.4
1	F	141	GLY	2.4
1	B	197	PRO	2.4
1	E	331	ARG	2.4
1	A	45	ALA	2.4
1	C	276	ILE	2.4
1	D	251	ASP	2.4
1	C	207	VAL	2.4
1	A	128	ALA	2.4
1	A	352	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	424	SER	2.4
1	A	35	VAL	2.4
1	A	419	VAL	2.4
1	D	311	ARG	2.4
1	A	270	LEU	2.4
1	C	275	ASP	2.4
1	C	415	SER	2.4
1	D	213	SER	2.4
1	C	240	VAL	2.4
1	C	371	ARG	2.4
1	C	476	PHE	2.4
1	D	157	VAL	2.4
1	E	384	ARG	2.4
1	F	442	GLU	2.4
1	B	283	THR	2.3
1	D	189	THR	2.3
1	E	135	LYS	2.3
1	F	310	SER	2.3
1	A	360	GLY	2.3
1	B	374	ASN	2.3
1	B	444	ILE	2.3
1	C	55	ILE	2.3
1	D	358	ILE	2.3
1	E	362	ILE	2.3
1	A	279	PHE	2.3
1	B	290	VAL	2.3
1	C	464	VAL	2.3
1	D	290	VAL	2.3
1	E	23	PHE	2.3
1	E	262	VAL	2.3
1	F	448	VAL	2.3
1	B	426	TRP	2.3
1	A	163	HIS	2.3
1	D	54	LYS	2.3
1	D	414	HIS	2.3
1	E	407	PRO	2.3
1	F	272	ASP	2.3
1	E	124	ILE	2.3
1	C	382	PHE	2.3
1	E	133	ASP	2.3
1	F	32	PRO	2.3
1	D	9	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	175	GLU	2.3
1	B	261	ASN	2.3
1	A	362	ILE	2.3
1	C	5	PHE	2.3
1	D	200	GLN	2.3
1	E	122	VAL	2.3
1	A	493	TRP	2.3
1	C	82	PRO	2.3
1	A	100	TYR	2.3
1	B	440	ALA	2.3
1	C	72	ALA	2.3
1	C	353	ALA	2.3
1	D	27	THR	2.3
1	E	429	ALA	2.3
1	F	302	ALA	2.3
1	E	205	LYS	2.3
1	E	484	LYS	2.3
1	F	205	LYS	2.3
1	B	428	VAL	2.3
1	A	303	SER	2.3
1	B	412	HIS	2.3
1	A	31	ASN	2.3
1	D	330	LEU	2.3
1	E	71	LEU	2.3
1	F	174	CYS	2.3
1	A	283	THR	2.3
1	C	81	THR	2.3
1	F	37	ALA	2.3
1	D	480	GLN	2.3
1	F	206	ILE	2.3
1	B	142	VAL	2.3
1	B	284	GLU	2.3
1	C	142	VAL	2.3
1	C	347	VAL	2.3
1	D	347	VAL	2.3
1	D	75	ASP	2.3
1	E	96	GLY	2.3
1	D	36	PRO	2.3
1	F	460	LEU	2.3
1	A	114	TYR	2.3
1	C	236	ALA	2.3
1	E	265	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	98	THR	2.3
1	E	113	ARG	2.3
1	A	220	ASP	2.3
1	C	300	LYS	2.3
1	D	172	ASP	2.3
1	E	195	GLY	2.3
1	A	424	SER	2.3
1	A	456	LEU	2.3
1	C	241	SER	2.3
1	E	267	LEU	2.3
1	A	81	THR	2.3
1	E	158	GLU	2.3
1	F	100	TYR	2.3
1	A	445	ASP	2.3
1	B	205	LYS	2.3
1	F	406	VAL	2.3
1	A	486	GLY	2.2
1	C	59	THR	2.2
1	E	439	ARG	2.2
1	E	463	GLY	2.2
1	F	195	GLY	2.2
1	F	463	GLY	2.2
1	B	191	SER	2.2
1	E	404	SER	2.2
1	F	249	PRO	2.2
1	F	481	GLU	2.2
1	C	325	LYS	2.2
1	C	468	THR	2.2
1	D	127	VAL	2.2
1	D	314	ILE	2.2
1	D	360	GLY	2.2
1	F	210	VAL	2.2
1	C	494	GLU	2.2
1	B	135	LYS	2.2
1	B	280	ASN	2.2
1	D	250	LYS	2.2
1	D	415	SER	2.2
1	E	441	HIS	2.2
1	B	236	ALA	2.2
1	F	204	ALA	2.2
1	B	98	THR	2.2
1	C	139	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	352	THR	2.2
1	D	430	ASP	2.2
1	E	473	ASP	2.2
1	E	22	GLY	2.2
1	E	58	PHE	2.2
1	A	266	VAL	2.2
1	C	124	ILE	2.2
1	D	209	VAL	2.2
1	D	406	VAL	2.2
1	E	421	VAL	2.2
1	E	443	ILE	2.2
1	A	305	CYS	2.2
1	B	213	SER	2.2
1	E	94	ASN	2.2
1	E	174	CYS	2.2
1	C	197	PRO	2.2
1	E	489	ARG	2.2
1	F	492	ARG	2.2
1	F	102	ASP	2.2
1	C	158	GLU	2.2
1	F	158	GLU	2.2
1	C	282	TYR	2.2
1	B	423	ILE	2.2
1	B	443	ILE	2.2
1	D	396	VAL	2.2
1	F	423	ILE	2.2
1	D	298	ARG	2.2
1	E	97	SER	2.2
1	F	384	ARG	2.2
1	E	449	HIS	2.2
1	B	493	TRP	2.2
1	D	123	ALA	2.2
1	A	325	LYS	2.2
1	B	48	GLU	2.2
1	B	50	GLY	2.2
1	B	68	ASP	2.2
1	E	7	THR	2.2
1	F	115	GLY	2.2
1	F	393	THR	2.2
1	B	405	PHE	2.2
1	C	188	TYR	2.2
1	E	100	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	79	PHE	2.2
1	A	124	ILE	2.2
1	A	155	ILE	2.2
1	A	403	SER	2.2
1	D	62	SER	2.2
1	D	259	VAL	2.2
1	F	306	SER	2.2
1	B	229	GLN	2.2
1	F	78	LYS	2.2
1	A	74	ALA	2.2
1	B	232	GLY	2.2
1	B	353	ALA	2.2
1	C	246	GLY	2.2
1	D	343	ARG	2.2
1	A	95	ASN	2.2
1	A	157	VAL	2.2
1	A	350	ILE	2.2
1	A	404	SER	2.2
1	B	259	VAL	2.2
1	D	312	SER	2.2
1	A	196	LYS	2.2
1	E	355	GLU	2.2
1	E	416	GLU	2.2
1	E	465	LYS	2.2
1	C	450	PRO	2.2
1	F	171	HIS	2.2
1	F	339	PRO	2.2
1	F	425	GLU	2.2
1	B	322	ASP	2.2
1	F	451	ASP	2.2
1	A	149	CYS	2.2
1	A	204	ALA	2.2
1	E	493	TRP	2.2
1	B	211	ARG	2.2
1	E	391	PHE	2.2
1	B	83	TYR	2.1
1	B	114	TYR	2.1
1	B	216	ASN	2.1
1	D	374	ASN	2.1
1	B	206	ILE	2.1
1	D	125	ILE	2.1
1	D	481	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	70	VAL	2.1
1	A	366	HIS	2.1
1	E	274	PRO	2.1
1	A	169	GLY	2.1
1	C	217	ASP	2.1
1	E	56	GLY	2.1
1	C	356	ALA	2.1
1	F	474	CYS	2.1
1	C	58	PHE	2.1
1	B	219	SER	2.1
1	C	213	SER	2.1
1	C	485	SER	2.1
1	F	358	ILE	2.1
1	A	164	PRO	2.1
1	A	450	PRO	2.1
1	B	145	LEU	2.1
1	B	482	LEU	2.1
1	D	173	LEU	2.1
1	F	436	PRO	2.1
1	F	469	PRO	2.1
1	A	269	ALA	2.1
1	B	61	ALA	2.1
1	A	426	TRP	2.1
1	D	484	LYS	2.1
1	E	283	THR	2.1
1	E	494	GLU	2.1
1	B	14	PHE	2.1
1	D	5	PHE	2.1
1	D	23	PHE	2.1
1	A	241	SER	2.1
1	F	364	SER	2.1
1	B	15	VAL	2.1
1	B	120	VAL	2.1
1	F	396	VAL	2.1
1	C	71	LEU	2.1
1	C	399	ASP	2.1
1	A	150	ARG	2.1
1	D	141	GLY	2.1
1	F	307	LEU	2.1
1	F	354	LEU	2.1
1	D	394	PRO	2.1
1	E	332	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	446	LYS	2.1
1	D	494	GLU	2.1
1	E	273	ASN	2.1
1	F	241	SER	2.1
1	A	409	VAL	2.1
1	B	136	ILE	2.1
1	B	293	LEU	2.1
1	C	388	VAL	2.1
1	D	100	TYR	2.1
1	D	288	ASP	2.1
1	E	293	LEU	2.1
1	E	316	ASP	2.1
1	F	111	ASP	2.1
1	B	190	PRO	2.1
1	E	32	PRO	2.1
1	F	242	GLU	2.1
1	D	46	ALA	2.1
1	E	382	PHE	2.1
1	B	162	LYS	2.1
1	A	44	ILE	2.1
1	B	144	ILE	2.1
1	D	448	VAL	2.1
1	D	282	TYR	2.1
1	D	459	TYR	2.1
1	E	299	ILE	2.1
1	F	145	LEU	2.1
1	A	27	THR	2.1
1	A	140	THR	2.1
1	A	392	THR	2.1
1	C	338	ASN	2.1
1	D	86	ASN	2.1
1	F	273	ASN	2.1
1	C	221	PHE	2.1
1	C	359	PHE	2.1
1	A	50	GLY	2.1
1	C	192	ASP	2.1
1	C	272	ASP	2.1
1	F	225	ASP	2.1
1	F	438	GLU	2.1
1	B	39	ILE	2.1
1	C	443	ILE	2.1
1	F	17	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	188	TYR	2.1
1	E	339	PRO	2.1
1	C	302	ALA	2.1
1	C	273	ASN	2.1
1	C	393	THR	2.1
1	D	131	THR	2.1
1	D	320	ASN	2.1
1	C	97	SER	2.1
1	D	85	SER	2.1
1	D	106	SER	2.1
1	D	438	GLU	2.1
1	E	288	ASP	2.1
1	A	6	ILE	2.1
1	B	44	ILE	2.1
1	C	414	HIS	2.1
1	A	447	CYS	2.1
1	C	474	CYS	2.1
1	E	247	ARG	2.1
1	E	298	ARG	2.1
1	E	374	ASN	2.1
1	F	453	ARG	2.1
1	D	107	THR	2.1
1	F	27	THR	2.1
1	F	355	GLU	2.1
1	A	377	GLY	2.1
1	B	252	PHE	2.1
1	F	279	PHE	2.1
1	B	431	LEU	2.0
1	C	307	LEU	2.0
1	A	148	ILE	2.0
1	A	317	ILE	2.0
1	A	348	ILE	2.0
1	B	86	ASN	2.0
1	C	46	ALA	2.0
1	C	154	ARG	2.0
1	F	42	ARG	2.0
1	E	490	ASN	2.0
1	F	86	ASN	2.0
1	A	85	SER	2.0
1	A	306	SER	2.0
1	C	102	ASP	2.0
1	C	161	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	486	GLY	2.0
1	E	5	PHE	2.0
1	D	482	LEU	2.0
1	C	199	VAL	2.0
1	B	299	ILE	2.0
1	D	198	TYR	2.0
1	E	452	TYR	2.0
1	B	51	ASN	2.0
1	E	264	ASN	2.0
1	E	356	ALA	2.0
1	F	216	ASN	2.0
1	A	49	LYS	2.0
1	C	364	SER	2.0
1	D	475	CYS	2.0
1	F	81	THR	2.0
1	A	315	GLN	2.0
1	D	301	PHE	2.0
1	E	238	PHE	2.0
1	E	359	PHE	2.0
1	C	362	ILE	2.0
1	E	166	GLU	2.0
1	B	18	ASN	2.0
1	A	68	ASP	2.0
1	B	85	SER	2.0
1	B	487	ASP	2.0
1	E	74	ALA	2.0
1	E	430	ASP	2.0
1	A	145	LEU	2.0
1	B	177	LEU	2.0
1	B	307	LEU	2.0
1	B	343	ARG	2.0
1	C	126	GLU	2.0
1	C	311	ARG	2.0
1	D	105	LEU	2.0
1	E	126	GLU	2.0
1	E	239	LEU	2.0
1	E	437	ARG	2.0
1	A	142	VAL	2.0
1	A	434	LYS	2.0
1	B	207	VAL	2.0
1	B	406	VAL	2.0
1	E	342	VAL	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	D	507	1/1	0.85	0.10	17,17,17,17	0
2	ZN	E	508	1/1	0.86	0.10	25,25,25,25	0
2	ZN	A	507	1/1	0.87	0.09	16,16,16,16	0
2	ZN	B	507	1/1	0.89	0.09	20,20,20,20	0
2	ZN	C	507	1/1	0.94	0.10	18,18,18,18	0
2	ZN	E	507	1/1	0.97	0.07	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.