



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:19 AM UTC

PDB ID : 2NVV / pdb_00002nvv
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

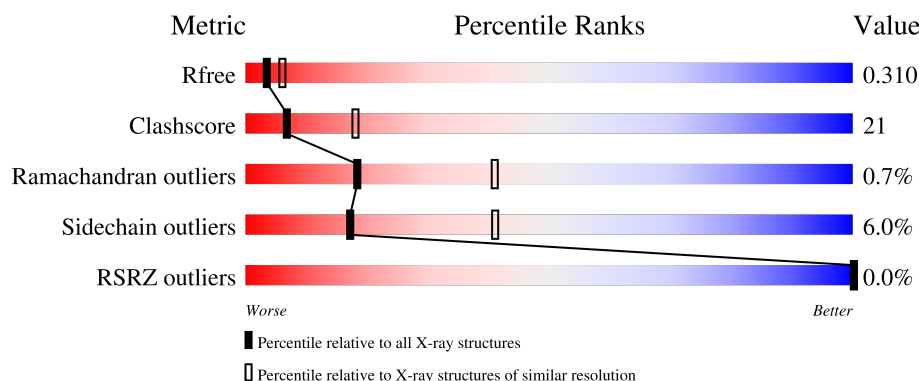
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

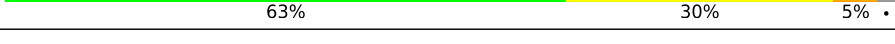
The reported resolution of this entry is 2.70 Å.

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of 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	
1	B	506	
1	C	506	
1	D	506	

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	E	506	59%33%6%•
1	F	506	58%33%6%•

2 Entry composition [i](#)

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
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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
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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

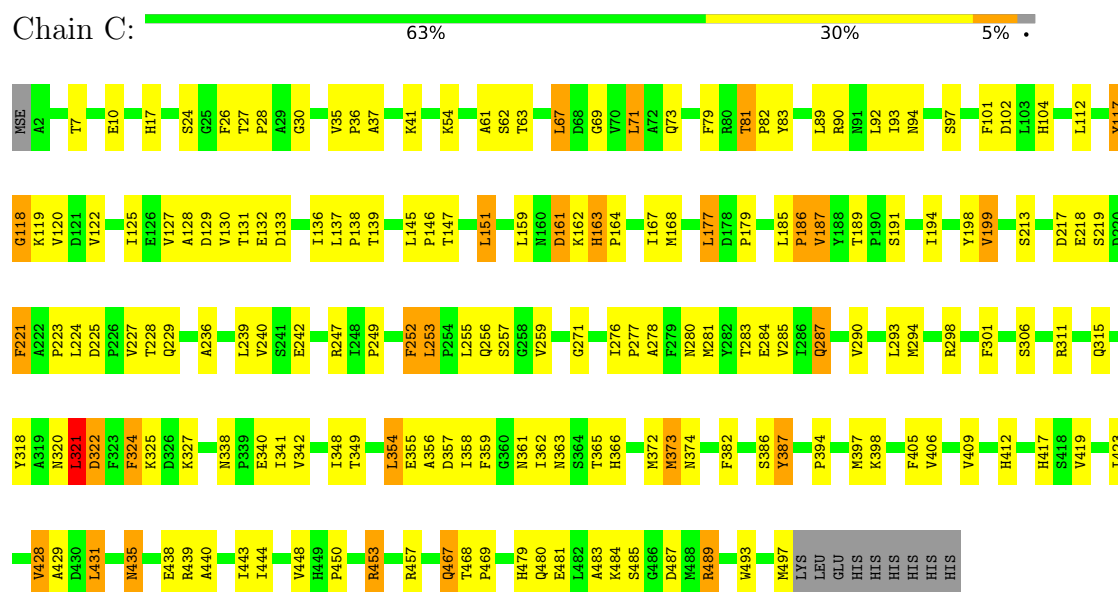
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

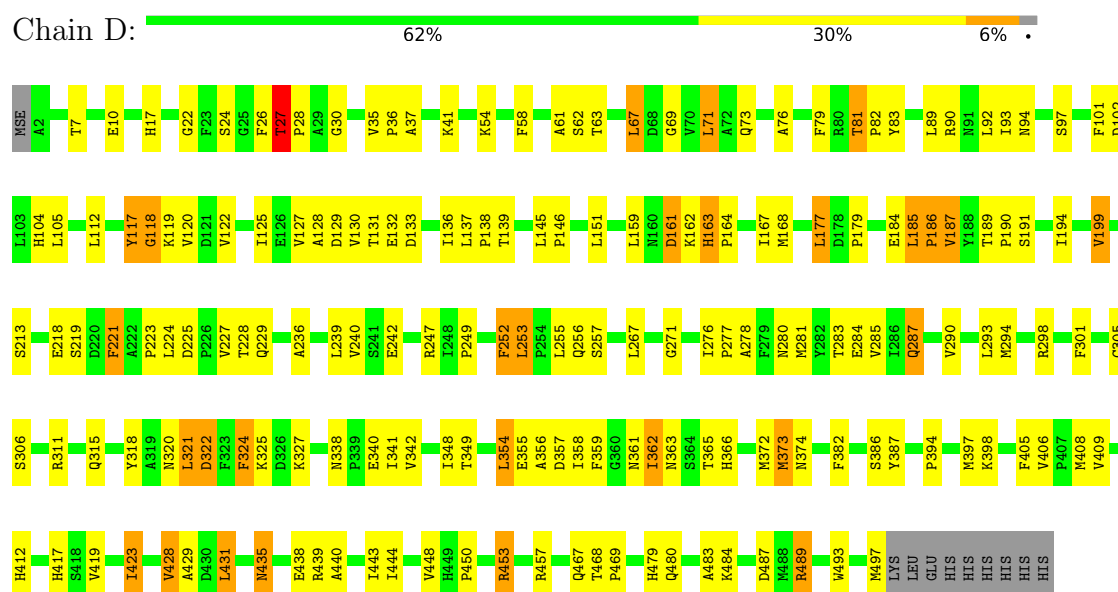
- Molecule 3 is water.

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

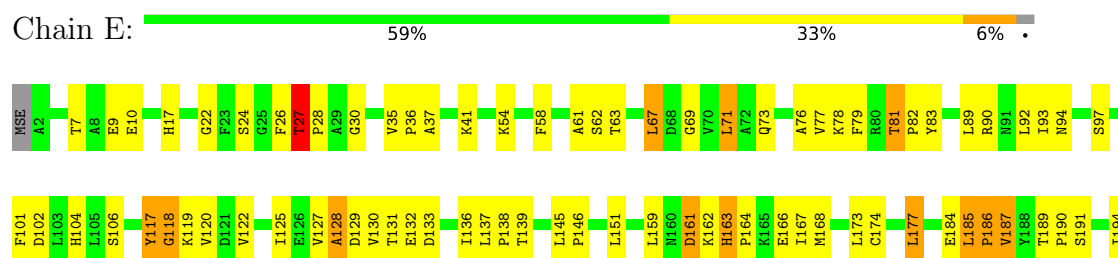
• Molecule 1: Acetyl-CoA hydrolase/transferase family protein

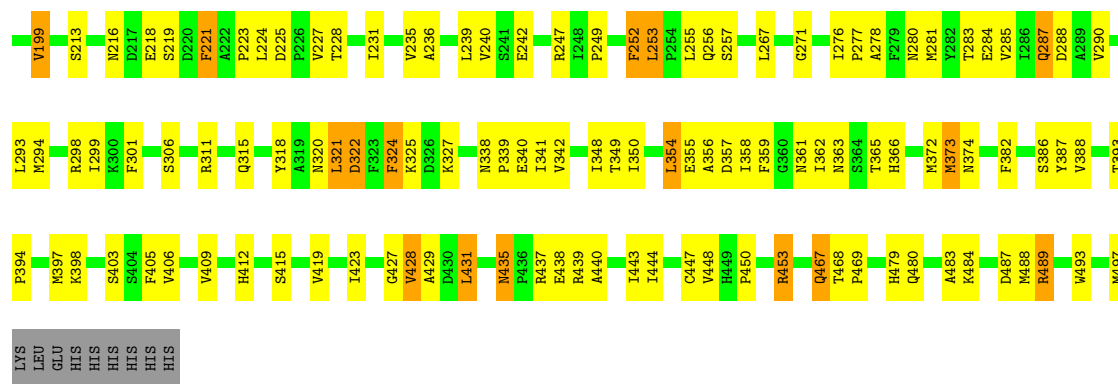


• Molecule 1: Acetyl-CoA hydrolase/transferase family protein



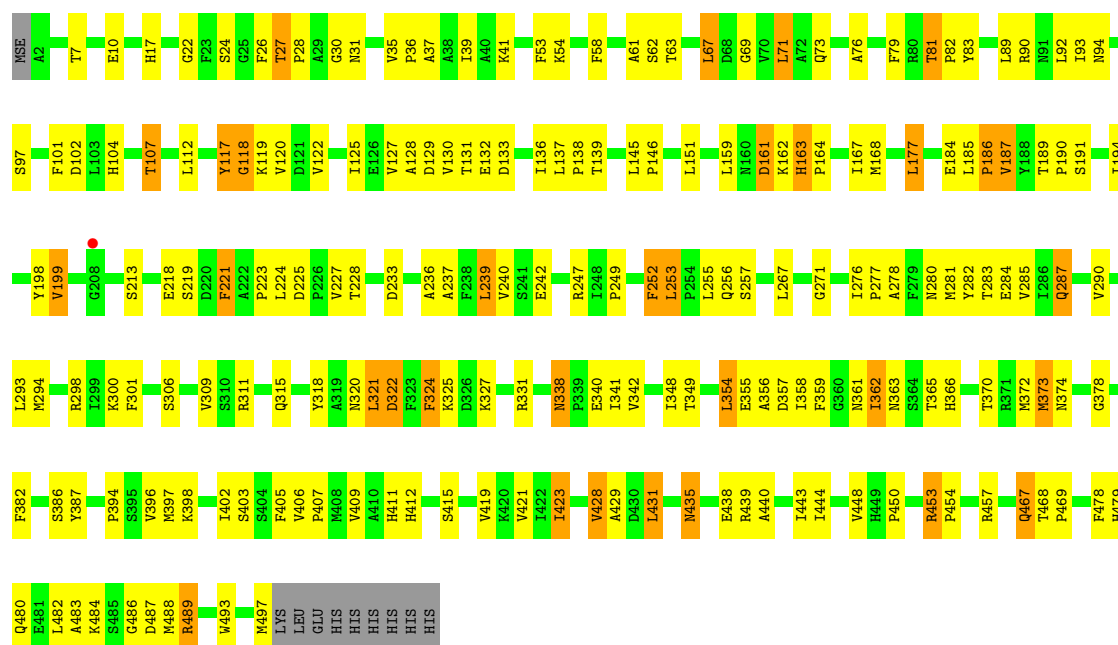
• Molecule 1: Acetyl-CoA hydrolase/transferase family protein





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

Chain F: 58% 33% 6% •



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 19.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.95-2.70) 52.4 (19.95-2.70)	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 0.306 , 0.310	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)	0.33 , 10.5	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	0.91	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/3898	1.00	16/5269 (0.3%)
1	B	0.46	0/3898	1.00	15/5269 (0.3%)
1	C	0.48	0/3898	1.00	15/5269 (0.3%)
1	D	0.47	0/3898	1.00	19/5269 (0.4%)
1	E	0.48	0/3898	0.99	13/5269 (0.2%)
1	F	0.48	0/3898	1.00	17/5269 (0.3%)
All	All	0.47	0/23388	1.00	95/31614 (0.3%)

There are no bond length outliers.

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	LEU	N-CA-C	-6.75	104.00	111.36
1	E	354	LEU	N-CA-C	-6.57	104.20	111.36
1	B	104	HIS	N-CA-C	-6.45	100.10	109.59
1	C	104	HIS	N-CA-C	-6.43	100.13	109.59
1	C	354	LEU	N-CA-C	-6.43	104.36	111.36
1	A	104	HIS	N-CA-C	-6.42	100.15	109.59
1	B	354	LEU	N-CA-C	-6.31	104.49	111.36
1	D	354	LEU	N-CA-C	-6.31	104.48	111.36
1	F	354	LEU	N-CA-C	-6.21	104.59	111.36
1	F	104	HIS	N-CA-C	-6.18	100.50	109.59
1	E	104	HIS	N-CA-C	-6.13	100.58	109.59
1	D	104	HIS	N-CA-C	-6.12	100.60	109.59
1	E	128	ALA	N-CA-C	-6.11	105.99	113.50
1	A	128	ALA	N-CA-C	-6.02	106.09	113.50
1	D	128	ALA	N-CA-C	-5.97	106.16	113.50
1	B	128	ALA	N-CA-C	-5.89	106.26	113.50
1	F	128	ALA	N-CA-C	-5.86	106.29	113.50
1	F	177	LEU	N-CA-C	-5.83	102.84	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	HIS	CA-C-N	5.83	125.59	119.76
1	C	163	HIS	C-N-CA	5.83	125.59	119.76
1	C	117	TYR	N-CA-C	-5.77	100.00	109.40
1	D	163	HIS	CA-C-N	5.76	125.53	119.76
1	D	163	HIS	C-N-CA	5.76	125.53	119.76
1	A	163	HIS	CA-C-N	5.75	125.66	119.85
1	A	163	HIS	C-N-CA	5.75	125.66	119.85
1	C	128	ALA	N-CA-C	-5.72	106.47	113.50
1	E	185	LEU	CA-C-N	5.70	126.97	119.84
1	E	185	LEU	C-N-CA	5.70	126.97	119.84
1	B	177	LEU	N-CA-C	-5.66	103.45	110.41
1	F	117	TYR	N-CA-C	-5.64	100.52	109.59
1	F	324	PHE	N-CA-C	5.63	119.33	112.23
1	C	177	LEU	N-CA-C	-5.63	103.10	110.53
1	A	117	TYR	N-CA-C	-5.58	100.31	109.40
1	E	177	LEU	N-CA-C	-5.53	103.22	110.53
1	B	117	TYR	N-CA-C	-5.51	100.41	109.40
1	E	324	PHE	N-CA-C	5.51	119.17	112.23
1	B	396	VAL	N-CA-C	5.49	115.51	108.82
1	A	177	LEU	N-CA-C	-5.48	103.29	110.53
1	C	387	TYR	N-CA-C	-5.48	105.21	111.07
1	D	117	TYR	N-CA-C	-5.48	100.47	109.40
1	D	177	LEU	N-CA-C	-5.47	103.68	110.41
1	D	366	HIS	N-CA-C	5.47	117.43	108.52
1	F	366	HIS	N-CA-C	5.46	117.62	108.73
1	A	324	PHE	N-CA-C	5.43	119.07	112.23
1	C	112	LEU	N-CA-C	-5.42	105.45	111.36
1	D	324	PHE	N-CA-C	5.42	118.36	111.69
1	D	162	LYS	N-CA-C	5.41	119.37	112.87
1	A	65	ALA	N-CA-C	-5.41	106.63	113.18
1	E	366	HIS	N-CA-C	5.41	117.54	108.73
1	A	366	HIS	N-CA-C	5.40	117.32	108.52
1	C	324	PHE	N-CA-C	5.38	119.01	112.23
1	A	162	LYS	N-CA-C	5.36	119.44	113.01
1	C	366	HIS	N-CA-C	5.35	117.24	108.52
1	C	162	LYS	N-CA-C	5.33	119.41	113.01
1	F	163	HIS	CA-C-N	5.33	125.09	119.76
1	F	163	HIS	C-N-CA	5.33	125.09	119.76
1	F	338	ASN	N-CA-C	5.31	117.31	109.50
1	F	112	LEU	N-CA-C	-5.31	105.41	111.14
1	D	105	LEU	N-CA-C	5.31	117.75	111.33
1	A	387	TYR	N-CA-C	-5.28	105.42	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	163	HIS	CA-C-N	5.27	125.18	119.85
1	E	163	HIS	C-N-CA	5.27	125.18	119.85
1	A	112	LEU	N-CA-C	-5.27	105.62	111.36
1	B	229	GLN	N-CA-C	-5.26	105.44	111.07
1	F	162	LYS	N-CA-C	5.24	119.30	113.01
1	D	112	LEU	N-CA-C	-5.24	105.65	111.36
1	E	27	THR	N-CA-C	-5.22	98.27	109.81
1	B	163	HIS	CA-C-N	5.22	124.98	119.76
1	B	163	HIS	C-N-CA	5.22	124.98	119.76
1	E	117	TYR	N-CA-C	-5.22	101.19	109.59
1	E	162	LYS	N-CA-C	5.22	119.27	113.01
1	D	362	ILE	N-CA-C	5.20	115.97	108.48
1	F	423	ILE	N-CA-C	5.20	115.77	108.17
1	F	362	ILE	N-CA-C	5.17	115.92	108.48
1	A	185	LEU	CA-C-N	5.17	126.30	119.84
1	A	185	LEU	C-N-CA	5.17	126.30	119.84
1	C	229	GLN	N-CA-C	-5.16	105.55	111.07
1	D	185	LEU	CA-C-N	5.15	126.28	119.84
1	D	185	LEU	C-N-CA	5.15	126.28	119.84
1	D	305	CYS	N-CA-C	-5.13	107.40	113.97
1	B	105	LEU	N-CA-C	5.10	117.50	111.33
1	B	162	LYS	N-CA-C	5.10	119.13	113.01
1	F	107	THR	N-CA-C	5.10	119.77	113.50
1	A	332	PRO	N-CA-C	-5.08	103.30	111.38
1	B	366	HIS	N-CA-C	5.08	116.81	108.52
1	C	321	LEU	N-CA-C	-5.05	106.22	112.38
1	B	332	PRO	N-CA-C	-5.05	103.36	111.38
1	F	387	TYR	N-CA-C	-5.04	105.67	111.07
1	B	112	LEU	N-CA-C	-5.04	105.86	111.36
1	F	396	VAL	N-CA-C	5.04	114.97	108.82
1	B	65	ALA	N-CA-C	-5.04	107.08	113.18
1	D	27	THR	N-CA-C	-5.04	98.67	109.81
1	D	423	ILE	N-CA-C	5.04	115.53	108.17
1	D	229	GLN	N-CA-C	-5.01	105.82	111.28
1	C	217	ASP	N-CA-C	-5.00	104.25	110.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3828	0	3808	160	0
1	B	3828	0	3808	158	0
1	C	3828	0	3808	155	0
1	D	3828	0	3808	160	0
1	E	3828	0	3808	177	0
1	F	3828	0	3808	195	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
3	A	30	0	0	10	0
3	B	22	0	0	9	0
3	C	30	0	0	2	0
3	D	23	0	0	2	0
3	E	52	0	0	20	0
3	F	47	0	0	30	0
All	All	23178	0	22848	981	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 (981) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:ASN:HD21	1:F:372:MSE:H	1.22	0.88
1:A:136:ILE:HB	1:A:199:VAL:HG13	1.52	0.88
1:E:365:THR:O	1:E:373:MSE:HB2	1.75	0.87
1:D:365:THR:O	1:D:373:MSE:HB2	1.74	0.87
1:E:94:ASN:HD21	1:E:372:MSE:H	1.21	0.87
1:B:136:ILE:HB	1:B:199:VAL:HG13	1.53	0.87
1:F:365:THR:O	1:F:373:MSE:HB2	1.74	0.86
1:F:127:VAL:HG12	1:F:129:ASP:H	1.42	0.85
1:A:340:GLU:HG3	1:B:340:GLU:HG3	1.58	0.85
1:A:127:VAL:HG12	1:A:129:ASP:H	1.42	0.84
1:F:17:HIS:HD2	1:F:54:LYS:H	1.25	0.84
1:B:36:PRO:HD2	3:B:513:HOH:O	1.75	0.84
1:E:447:CYS:HB2	3:E:541:HOH:O	1.77	0.84
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:HG22	1:A:82:PRO:HA	1.65	0.78
1:A:450:PRO:HA	1:A:453:ARG:HG3	1.65	0.78
1:B:81:THR:HG22	1:B:82:PRO:HA	1.66	0.78
1:F:450:PRO:HA	1:F:453:ARG:HG3	1.65	0.78
1:C:81:THR:HG22	1:C:82:PRO:HA	1.65	0.78
1:F:370:THR:HG23	3:F:550:HOH:O	1.85	0.77
1:F:480:GLN:O	1:F:484:LYS:HG2	1.83	0.77
1:E:435:ASN:HD21	1:E:438:GLU:HG3	1.50	0.77
1:C:340:GLU:HG3	1:D:340:GLU:HG3	1.66	0.77
1:C:493:TRP:O	1:C:497:MSE:HG2	1.85	0.76
1:A:127:VAL:HG12	1:A:129:ASP:N	1.99	0.76
1:E:340:GLU:HG3	1:F:340:GLU:HG3	1.67	0.76
1:E:81:THR:HG22	1:E:82:PRO:HA	1.68	0.76
1: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:293:LEU:HD22	1:F:298:ARG:HG2	1.69	0.74
1:F:294:MSE:HE3	1:F:327:LYS:HB2	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:E:545:HOH:O	1:F:415:SER:HB2	1.91	0.71
1:F:256:GLN:HA	1:F:283:THR:HG22	1.73	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:435:ASN:C	1:C:435:ASN:HD22	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:163:HIS:HD2	1:F:318:TYR:OH	1.79	0.64
1:F:294:MSE:HE2	1:F:324:PHE:CD2	2.33	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
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:26:PHE:HB3	1:B:306:SER:HB3	1.80	0.63
1:B:287:GLN:HE21	1:B:287:GLN:H	1.46	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:B:435:ASN:C	1:B:435:ASN:HD22	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:VAL:CG1	1:B:341:ILE:HD12	2.30	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: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
1:A:256:GLN:HA	1:A:283:THR:HG23	1.82	0.61
1:D:287:GLN:H	1:D:287:GLN:HE21	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:A:435:ASN:C	1:A:435:ASN:HD22	2.07	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:E:435:ASN:C	1:E:435:ASN:HD22	2.09	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:94:ASN:HD21	1:C:372:MSE:N	1.94	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: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:F:435:ASN:C	1:F:435:ASN:HD22	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:483:ALA:HB3	1:E:484:LYS:HE3	1.84	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
1:C:256:GLN:HA	1:C:283:THR:HG23	1.82	0.59
1:C:435:ASN:ND2	1:C:435:ASN:C	2.61	0.59
1:D:435:ASN:C	1:D:435:ASN:HD22	2.09	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: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: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:H	1:B:287:GLN:NE2	2.02	0.58
1:F:435:ASN:HD21	1:F:438:GLU:H	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:225:ASP:OD2	1:B:228:THR:HG23	2.05	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: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:C:82:PRO:O	1:C:102:ASP:HA	2.06	0.56
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: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:77:VAL:HG22	3:E:555:HOH:O	2.05	0.55
1:E:487:ASP:OD1	1:E:489:ARG:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:PHE:O	1:A:439:ARG:HD2	2.06	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: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:A:435:ASN:ND2	1:A:435:ASN:C	2.65	0.54
1:B:36:PRO:HG3	1:B:67:LEU:HD22	1.89	0.54
1:D:90:ARG:HD3	1:D:373:MSE:O	2.06	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: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:E:216:ASN:ND2	3:E:538:HOH:O	2.40	0.54
1:D:249:PRO:HG2	1:D:253:LEU:HD13	1.88	0.54
1:B:349:THR:HG23	1:B:386:SER:HB3	1.90	0.54
1:D:487:ASP:OD1	1:D:489:ARG:HD3	2.07	0.54
1:F:81:THR:HG22	1:F:82:PRO:CA	2.36	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: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:92:LEU:HD12	1:A:97:SER:HB2	1.90	0.54
1:A:127:VAL:HG13	1:A:137:LEU:O	2.08	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:81:THR:HG22	1:D:82:PRO:CA	2.36	0.54
1:D:130:VAL:HG13	1:D:130:VAL:O	2.08	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:435:ASN:ND2	1:D:435:ASN:C	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:435:ASN:ND2	1:B:435:ASN:C	2.66	0.53
1:B:294:MSE:CE	1:B:327:LYS:HB2	2.39	0.53
1:B:361:ASN:C	1:B:362:ILE:HD12	2.33	0.53
1:D:117:TYR:O	1:D:118:GLY:O	2.27	0.53
1:D:287:GLN:H	1:D:287:GLN:NE2	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
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:H	1:F:287:GLN:HE21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:320:ASN:HA	1:F:322:ASP:OD1	2.10	0.51
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:C:361:ASN:C	1:C:362:ILE:HD12	2.35	0.51
1:D:36:PRO:HG3	1:D:67:LEU:HD22	1.91	0.51
1:F:79:PHE:CD1	1:F:79:PHE:C	2.89	0.51
1:F:131:THR:CG2	1:F:133:ASP:OD1	2.58	0.51
1:D:361:ASN:C	1:D:362:ILE:HD12	2.36	0.51
1:C:127:VAL:HG13	1:C:137:LEU:O	2.11	0.51
1:D:79:PHE:CD1	1:D:79:PHE:C	2.89	0.51
1:D:338:ASN:O	1:D:342:VAL:HG23	2.11	0.51
1:E:79:PHE:CD1	1:E:79:PHE:C	2.89	0.51
1:E:435:ASN:ND2	1:E:435:ASN:C	2.65	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:255:LEU:HD23	1:A:348:ILE:HB	1.92	0.50
1:A:256:GLN:HG3	1:A:382:PHE:CE1	2.47	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: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
1:F:435:ASN:ND2	1:F:435:ASN:C	2.66	0.50
1:A:440:ALA:O	1:A:444:ILE:HG13	2.12	0.50
1:E:130:VAL:HG13	1:E:130:VAL:O	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: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:27:THR:O	1:C:28:PRO:C	2.55	0.49
1:C:281:MSE:HE3	1:C:283:THR:CG2	2.42	0.49
1:A:37:ALA:HB2	3:A:519:HOH:O	2.12	0.49
1:A:131:THR:CG2	1:A:133:ASP:OD1	2.60	0.49
1:D:255:LEU:HD23	1:D:348:ILE:HB	1.92	0.49
1:B:79:PHE:CD1	1:B:79:PHE:C	2.90	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:A:361:ASN:C	1:A:362:ILE:HD12	2.38	0.49
1:C:130:VAL:O	1:C:130:VAL:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:79:PHE:CD1	1:A:79:PHE:C	2.91	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: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:HG13	1:F:130:VAL:O	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: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
1:A:397:MSE:HG2	1:A:398:LYS:N	2.28	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:35:VAL:N	1:B:36:PRO:HD2	2.29	0.48
1:B:131:THR:HG22	1:B:132:GLU:N	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: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:69:GLY:O	1:C:73:GLN:HG3	2.13	0.48
1:C:293:LEU:O	1:C:298:ARG:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:440:ALA:O	1:E:444:ILE:HG13	2.14	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:69:GLY:O	1:D:73:GLN:HG3	2.14	0.48
1:D:280:ASN:HD22	1:D:301:PHE:HB3	1.78	0.48
1:A:27:THR:O	1:A:28:PRO:C	2.57	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
1:A:69:GLY:O	1:A:73:GLN:HG3	2.14	0.48
1:C:89:LEU:O	1:C:93:ILE:HG13	2.13	0.48
1:C:349:THR:CG2	1:C:386:SER:HB3	2.44	0.48
1:D:131:THR:HG22	1:D:132:GLU:N	2.29	0.48
1: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:F:361:ASN:C	1:F:362:ILE:HD12	2.38	0.47
1:B:67:LEU:O	1:B:71:LEU:HB2	2.14	0.47
1:C:94:ASN:HD22	1:D:467:GLN:H	1.61	0.47
1:C:320:ASN:HA	1:C:322:ASP:OD1	2.13	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:35:VAL:N	1:E:36:PRO:HD2	2.30	0.47
1:E:221:PHE:CZ	1:E:223:PRO:HG3	2.50	0.47
1:F:27:THR:HA	1:F:62:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:89:LEU:O	1:B:93:ILE:HG13	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: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: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:F:294:MSE:CE	1:F:327:LYS:HB2	2.39	0.47
1:C:92:LEU:CD1	1:C:97:SER:HB2	2.45	0.47
1:C:481:GLU:OE1	1:C:485:SER:OG	2.30	0.47
1:E:361:ASN:C	1:E:362:ILE:HD12	2.40	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:C:79:PHE:CD1	1:C:79:PHE:C	2.92	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:O	1:A:130:VAL:HG13	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
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: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:69:GLY:O	1:B:73:GLN:HG3	2.15	0.46
1:B:440:ALA:O	1:B:444:ILE:HG13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ASN:HD22	1:C:301:PHE:HB3	1.80	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: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:27:THR:HA	1:D:62:SER:OG	2.14	0.46
1:D:36:PRO:HG2	3:D:512:HOH:O	2.16	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: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
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: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:D:271:GLY:HA2	1:D:298:ARG:CD	2.46	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:27:THR:O	1:B:28:PRO:C	2.56	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:37:ALA:O	1:B:41:LYS:HG2	2.16	0.45
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:C:26:PHE:C	1:C:27:THR:HG23	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:F:26:PHE:CE1	1:F:61:ALA:HB2	2.50	0.45
1:F:27:THR:O	1:F:28:PRO:C	2.57	0.45
1:F:221:PHE:CE1	1:F:223:PRO:HD3	2.51	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
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:35:VAL:N	1:C:36:PRO:HD2	2.32	0.45
1:C:271:GLY:HA2	1:C:298:ARG:CD	2.47	0.45
1:A:26:PHE:C	1:A:27:THR:HG23	2.42	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:E:37:ALA:O	1:E:41:LYS:HG2	2.17	0.45
1:C:83:TYR:CZ	1:C:374:ASN:HB3	2.52	0.45
1:D:27:THR:O	1:D:28:PRO:C	2.60	0.45
1:D:435:ASN:ND2	1:D:438:GLU:CG	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:PHE:C	1:F:27:THR:HG23	2.41	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:D:37:ALA:O	1:D:41:LYS:HG2	2.17	0.44
1:D:221:PHE:CE1	1:D:223:PRO:HD3	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:TYR:CZ	1:B:374:ASN:HB3	2.53	0.43
1:B:252:PHE:HB2	1:B:277:PRO:HG2	2.00	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:277:PRO:O	1:A:278:ALA:C	2.61	0.43
1:A:357:ASP:N	3:A:536:HOH:O	2.51	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:92:LEU:CD1	1:D:97:SER:HB2	2.48	0.43
1:D:256:GLN:CA	1:D:283:THR:HG22	2.46	0.43
1:F:331:ARG:CZ	3:F:527:HOH:O	2.66	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
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:26:PHE:C	1:E:27:THR:HG23	2.44	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:B:198:TYR:CD1	1:B:198:TYR:C	2.97	0.43
1:C:145:LEU:HB3	1:C:146:PRO:CD	2.49	0.43
1:D:26:PHE:C	1:D:27:THR:HG23	2.44	0.43
1:D:277:PRO:O	1:D:278:ALA:C	2.61	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:63:THR:HB	1:F:67:LEU:HG	2.00	0.43
1:F:138:PRO:HG3	1:F:145:LEU:HD21	2.01	0.43
1:A:89:LEU:O	1:A:93:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:417:HIS:HE1	1:D:102:ASP:CG	2.26	0.43
1:C:468:THR:HA	1:C:469:PRO:HD3	1.84	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:167:ILE:O	1:F:168:MSE:C	2.62	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:C:467:GLN:N	1:D:94:ASN:HD22	2.14	0.43
1:D:227:VAL:HG11	1:D:394:PRO:HB3	2.01	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:C:277:PRO:O	1:C:278:ALA:C	2.62	0.42
1:F:397:MSE:HB3	1:F:402:ILE:HB	2.01	0.42
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:F:277:PRO:O	1:F:278:ALA:C	2.62	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:92:LEU:CD1	1:E:97:SER:HB2	2.49	0.42
1:E:136:ILE:HD12	1:E:136:ILE:N	2.34	0.42
1:A:340:GLU:CD	1:B:340:GLU:HG3	2.44	0.42
1:B:63:THR:HB	1:B:67:LEU:HG	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ASN:ND2	1:D:372:MSE:H	2.01	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:26:PHE:C	1:B:27:THR:HG23	2.43	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:E:27:THR:O	1:E:28:PRO:C	2.62	0.42
1:E:277:PRO:O	1:E:278:ALA:C	2.62	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:37:ALA:O	1:C:41:LYS:HG2	2.19	0.42
1:C:252:PHE:HB2	1:C:277:PRO:HG2	2.02	0.42
1:D:267:LEU:O	1:D:293:LEU:HD11	2.20	0.42
1:D:287:GLN:NE2	1:D:290:VAL:HG23	2.35	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
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:102:ASP:CG	1:D:417:HIS:HE1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:340:GLU:HG3	1:B:340:GLU:CD	2.45	0.41
1:B:22:GLY:HA2	1:B:58:PHE:O	2.20	0.41
1:C:198:TYR:CD1	1:C:198:TYR:C	2.99	0.41
1:D:83:TYR:CZ	1:D:374:ASN:HB3	2.56	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: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:N	1:B:136:ILE:HD12	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:83:TYR:CZ	1:E:374:ASN:HB3	2.55	0.41
1:E:184:GLU:O	1:E:186:PRO:HD3	2.20	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:F:131:THR:HG22	1:F:133:ASP:H	1.85	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
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:63:THR:OG1	1:E:67:LEU:HB3	2.20	0.41
1:E:293:LEU:HD22	1:E:298:ARG:CG	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:VAL:HG11	1:B:394:PRO:HB3	2.03	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: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:167:ILE:O	1:C:168:MSE:C	2.64	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: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: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:26:PHE:O	1:F:27:THR:HG23	2.21	0.41
1:F:136:ILE:N	1:F:136:ILE:HD12	2.35	0.41
1:F:221:PHE:CD1	1:F:223:PRO:HD3	2.55	0.41
1:F:239:LEU:HD12	1:F:239:LEU:HA	1.84	0.41
1:D:102:ASP:OD2	1:D:102:ASP:N	2.51	0.41
1:E:256:GLN:CA	1:E:283:THR:HG22	2.45	0.41
1:F:167:ILE:HD13	1:F:167:ILE:HA	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:D:167:ILE:O	1:D:168:MSE:C	2.63	0.40
1:E:22:GLY:HA2	1:E:58:PHE:O	2.21	0.40
1:E:163:HIS:HA	1:E:164:PRO:HD2	1.93	0.40
1:E:468:THR:HA	1:E:469:PRO:HD3	1.85	0.40
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:167:ILE:O	1:E:168:MSE:C	2.63	0.40
1:E:231:ILE:O	1:E:235:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:198:TYR:CD1	1:F:198:TYR:C	2.99	0.40
1:A:22:GLY:HA2	1:A:58:PHE:O	2.21	0.40
1:A:131:THR:HG22	1:A:133:ASP:H	1.85	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:A:167:ILE:O	1:A:168:MSE:C	2.64	0.40
1:A:198:TYR:CD1	1:A:198:TYR:C	2.99	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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/506 (98%)	458 (93%)	33 (7%)	3 (1%)	21	44
1	B	494/506 (98%)	462 (94%)	29 (6%)	3 (1%)	21	44
1	C	494/506 (98%)	460 (93%)	31 (6%)	3 (1%)	21	44
1	D	494/506 (98%)	461 (93%)	29 (6%)	4 (1%)	16	37
1	E	494/506 (98%)	461 (93%)	29 (6%)	4 (1%)	16	37
1	F	494/506 (98%)	460 (93%)	30 (6%)	4 (1%)	16	37
All	All	2964/3036 (98%)	2762 (93%)	181 (6%)	21 (1%)	18	41

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%)	390 (94%)	26 (6%)	16	39
1	B	416/413 (101%)	392 (94%)	24 (6%)	18	42
1	C	416/413 (101%)	391 (94%)	25 (6%)	17	41
1	D	416/413 (101%)	392 (94%)	24 (6%)	18	42
1	E	416/413 (101%)	391 (94%)	25 (6%)	17	41
1	F	416/413 (101%)	391 (94%)	25 (6%)	17	41
All	All	2496/2478 (101%)	2347 (94%)	149 (6%)	17	41

All (149) 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	187	VAL
1	A	199	VAL
1	A	224	LEU
1	A	239	LEU
1	A	252	PHE
1	A	253	LEU
1	A	285	VAL
1	A	287	GLN
1	A	321	LEU
1	A	322	ASP
1	A	373	MSE
1	A	428	VAL
1	A	431	LEU
1	A	435	ASN
1	A	450	PRO
1	A	453	ARG
1	A	467	GLN
1	A	489	ARG
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	187	VAL
1	B	199	VAL
1	B	224	LEU
1	B	239	LEU
1	B	252	PHE
1	B	253	LEU
1	B	285	VAL
1	B	287	GLN
1	B	321	LEU
1	B	322	ASP
1	B	373	MSE
1	B	428	VAL
1	B	431	LEU
1	B	435	ASN
1	B	453	ARG
1	B	489	ARG
1	C	67	LEU
1	C	71	LEU
1	C	81	THR
1	C	122	VAL
1	C	151	LEU
1	C	159	LEU
1	C	161	ASP
1	C	177	LEU
1	C	187	VAL
1	C	199	VAL
1	C	224	LEU
1	C	239	LEU
1	C	252	PHE
1	C	253	LEU
1	C	285	VAL
1	C	287	GLN
1	C	321	LEU
1	C	322	ASP
1	C	373	MSE
1	C	428	VAL
1	C	431	LEU
1	C	435	ASN

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Mol	Chain	Res	Type
1	C	453	ARG
1	C	467	GLN
1	C	489	ARG
1	D	67	LEU
1	D	71	LEU
1	D	81	THR
1	D	122	VAL
1	D	151	LEU
1	D	159	LEU
1	D	161	ASP
1	D	177	LEU
1	D	187	VAL
1	D	199	VAL
1	D	224	LEU
1	D	239	LEU
1	D	252	PHE
1	D	253	LEU
1	D	285	VAL
1	D	287	GLN
1	D	321	LEU
1	D	322	ASP
1	D	373	MSE
1	D	428	VAL
1	D	431	LEU
1	D	435	ASN
1	D	453	ARG
1	D	489	ARG
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	187	VAL
1	E	199	VAL
1	E	224	LEU
1	E	239	LEU
1	E	252	PHE
1	E	253	LEU
1	E	285	VAL

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Mol	Chain	Res	Type
1	E	287	GLN
1	E	321	LEU
1	E	322	ASP
1	E	373	MSE
1	E	428	VAL
1	E	431	LEU
1	E	435	ASN
1	E	453	ARG
1	E	467	GLN
1	E	489	ARG
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	187	VAL
1	F	199	VAL
1	F	224	LEU
1	F	239	LEU
1	F	252	PHE
1	F	253	LEU
1	F	285	VAL
1	F	287	GLN
1	F	321	LEU
1	F	322	ASP
1	F	373	MSE
1	F	428	VAL
1	F	431	LEU
1	F	435	ASN
1	F	453	ARG
1	F	467	GLN
1	F	489	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	51	ASN
1	A	91	ASN

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Mol	Chain	Res	Type
1	A	94	ASN
1	A	95	ASN
1	A	104	HIS
1	A	163	HIS
1	A	200	GLN
1	A	261	ASN
1	A	264	ASN
1	A	280	ASN
1	A	287	GLN
1	A	374	ASN
1	A	385	ASN
1	A	414	HIS
1	A	435	ASN
1	A	467	GLN
1	A	479	HIS
1	A	480	GLN
1	B	17	HIS
1	B	51	ASN
1	B	91	ASN
1	B	94	ASN
1	B	95	ASN
1	B	104	HIS
1	B	163	HIS
1	B	200	GLN
1	B	216	ASN
1	B	261	ASN
1	B	264	ASN
1	B	280	ASN
1	B	287	GLN
1	B	374	ASN
1	B	385	ASN
1	B	412	HIS
1	B	435	ASN
1	B	441	HIS
1	B	467	GLN
1	B	480	GLN
1	C	17	HIS
1	C	31	ASN
1	C	51	ASN
1	C	91	ASN
1	C	94	ASN
1	C	95	ASN

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Mol	Chain	Res	Type
1	C	104	HIS
1	C	163	HIS
1	C	200	GLN
1	C	261	ASN
1	C	264	ASN
1	C	280	ASN
1	C	287	GLN
1	C	374	ASN
1	C	414	HIS
1	C	417	HIS
1	C	435	ASN
1	C	441	HIS
1	C	458	GLN
1	C	467	GLN
1	C	479	HIS
1	C	480	GLN
1	D	17	HIS
1	D	51	ASN
1	D	73	GLN
1	D	91	ASN
1	D	94	ASN
1	D	95	ASN
1	D	104	HIS
1	D	163	HIS
1	D	200	GLN
1	D	261	ASN
1	D	264	ASN
1	D	280	ASN
1	D	287	GLN
1	D	374	ASN
1	D	385	ASN
1	D	412	HIS
1	D	414	HIS
1	D	435	ASN
1	D	467	GLN
1	D	479	HIS
1	D	480	GLN
1	E	17	HIS
1	E	51	ASN
1	E	91	ASN
1	E	94	ASN
1	E	95	ASN

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Mol	Chain	Res	Type
1	E	163	HIS
1	E	200	GLN
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	385	ASN
1	E	414	HIS
1	E	435	ASN
1	E	458	GLN
1	E	467	GLN
1	E	479	HIS
1	E	480	GLN
1	F	17	HIS
1	F	51	ASN
1	F	91	ASN
1	F	94	ASN
1	F	95	ASN
1	F	104	HIS
1	F	163	HIS
1	F	200	GLN
1	F	261	ASN
1	F	264	ASN
1	F	280	ASN
1	F	287	GLN
1	F	374	ASN
1	F	414	HIS
1	F	417	HIS
1	F	435	ASN
1	F	467	GLN
1	F	479	HIS
1	F	480	GLN

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9	
1	A	484/506 (95%)	-1.09	0	100	100	6, 7, 18, 30	0
1	B	484/506 (95%)	-1.09	0	100	100	6, 7, 18, 30	0
1	C	484/506 (95%)	-1.08	0	100	100	6, 7, 18, 30	0
1	D	484/506 (95%)	-1.04	0	100	100	6, 7, 18, 30	0
1	E	484/506 (95%)	-0.93	0	100	100	6, 7, 18, 30	0
1	F	484/506 (95%)	-0.91	1 (0%)	91	90	6, 7, 18, 30	0
All	All	2904/3036 (95%)	-1.02	1 (0%)	100	100	6, 7, 18, 30	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	208	GLY	2.4

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	ZN	E	508	1/1	0.98	0.05	25,25,25,25	0
2	ZN	C	507	1/1	0.99	0.02	18,18,18,18	0
2	ZN	E	507	1/1	0.99	0.02	15,15,15,15	0
2	ZN	B	507	1/1	0.99	0.02	20,20,20,20	0
2	ZN	A	507	1/1	1.00	0.01	16,16,16,16	0
2	ZN	D	507	1/1	1.00	0.01	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.