



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2026 – 06:11 PM JST

PDB ID : 9VAG / pdb_00009vag
Title : Crystal structure of CoA transferase from *Thermus thermophilus*
Authors : Yoshida, A.; Yamamoto, H.; Nishiyama, M.
Deposited on : 2025-06-03
Resolution : 2.63 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
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)
Validation Pipeline (wwPDB-VP)	:	2.49

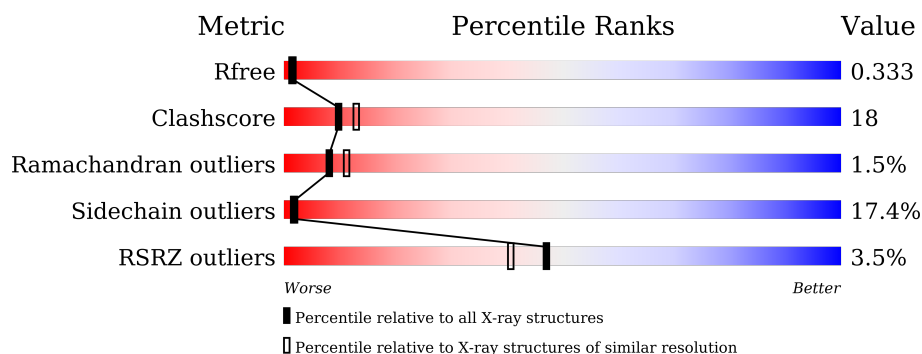
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	450	<div> <div>3%</div> <div> <div>55%</div> <div>29%</div> <div>9%</div> <div>• 5%</div> </div> </div>
1	B	450	<div> <div>2%</div> <div> <div>52%</div> <div>27%</div> <div>13%</div> <div>• 6%</div> </div> </div>
1	C	450	<div> <div>3%</div> <div> <div>50%</div> <div>30%</div> <div>11%</div> <div>• 6%</div> </div> </div>
1	D	450	<div> <div>4%</div> <div> <div>54%</div> <div>28%</div> <div>10%</div> <div>• 6%</div> </div> </div>
1	E	450	<div> <div>4%</div> <div> <div>54%</div> <div>28%</div> <div>9%</div> <div>• 6%</div> </div> </div>
1	F	450	<div> <div>3%</div> <div> <div>53%</div> <div>29%</div> <div>10%</div> <div>• 6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	450	<div><div>5%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>50%</div><div>31%</div><div>11%</div><div>•</div><div>6%</div></div>
1	H	450	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>52%</div><div>30%</div><div>9%</div><div>•</div><div>6%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25802 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 4-hydroxybutyrate coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	422	Total	C	N	O	S	0	0	0
			3216	2048	574	584	10			
1	H	423	Total	C	N	O	S	0	0	0
			3206	2041	574	581	10			
1	A	426	Total	C	N	O	S	0	3	0
			3277	2086	589	592	10			
1	B	422	Total	C	N	O	S	0	0	0
			3197	2031	574	582	10			
1	C	422	Total	C	N	O	S	0	2	0
			3226	2052	577	587	10			
1	D	423	Total	C	N	O	S	0	0	0
			3217	2050	572	585	10			
1	E	421	Total	C	N	O	S	0	1	0
			3196	2035	571	580	10			
1	G	424	Total	C	N	O	S	0	0	0
			3211	2047	570	584	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	445	HIS	-	expression tag	UNP Q72IP9
F	446	HIS	-	expression tag	UNP Q72IP9
F	447	HIS	-	expression tag	UNP Q72IP9
F	448	HIS	-	expression tag	UNP Q72IP9
F	449	HIS	-	expression tag	UNP Q72IP9
F	450	HIS	-	expression tag	UNP Q72IP9
H	445	HIS	-	expression tag	UNP Q72IP9
H	446	HIS	-	expression tag	UNP Q72IP9
H	447	HIS	-	expression tag	UNP Q72IP9
H	448	HIS	-	expression tag	UNP Q72IP9
H	449	HIS	-	expression tag	UNP Q72IP9
H	450	HIS	-	expression tag	UNP Q72IP9
A	445	HIS	-	expression tag	UNP Q72IP9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	446	HIS	-	expression tag	UNP Q72IP9
A	447	HIS	-	expression tag	UNP Q72IP9
A	448	HIS	-	expression tag	UNP Q72IP9
A	449	HIS	-	expression tag	UNP Q72IP9
A	450	HIS	-	expression tag	UNP Q72IP9
B	445	HIS	-	expression tag	UNP Q72IP9
B	446	HIS	-	expression tag	UNP Q72IP9
B	447	HIS	-	expression tag	UNP Q72IP9
B	448	HIS	-	expression tag	UNP Q72IP9
B	449	HIS	-	expression tag	UNP Q72IP9
B	450	HIS	-	expression tag	UNP Q72IP9
C	445	HIS	-	expression tag	UNP Q72IP9
C	446	HIS	-	expression tag	UNP Q72IP9
C	447	HIS	-	expression tag	UNP Q72IP9
C	448	HIS	-	expression tag	UNP Q72IP9
C	449	HIS	-	expression tag	UNP Q72IP9
C	450	HIS	-	expression tag	UNP Q72IP9
D	445	HIS	-	expression tag	UNP Q72IP9
D	446	HIS	-	expression tag	UNP Q72IP9
D	447	HIS	-	expression tag	UNP Q72IP9
D	448	HIS	-	expression tag	UNP Q72IP9
D	449	HIS	-	expression tag	UNP Q72IP9
D	450	HIS	-	expression tag	UNP Q72IP9
E	445	HIS	-	expression tag	UNP Q72IP9
E	446	HIS	-	expression tag	UNP Q72IP9
E	447	HIS	-	expression tag	UNP Q72IP9
E	448	HIS	-	expression tag	UNP Q72IP9
E	449	HIS	-	expression tag	UNP Q72IP9
E	450	HIS	-	expression tag	UNP Q72IP9
G	445	HIS	-	expression tag	UNP Q72IP9
G	446	HIS	-	expression tag	UNP Q72IP9
G	447	HIS	-	expression tag	UNP Q72IP9
G	448	HIS	-	expression tag	UNP Q72IP9
G	449	HIS	-	expression tag	UNP Q72IP9
G	450	HIS	-	expression tag	UNP Q72IP9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total O 1 1	0	0
2	A	11	Total O 11 11	0	0

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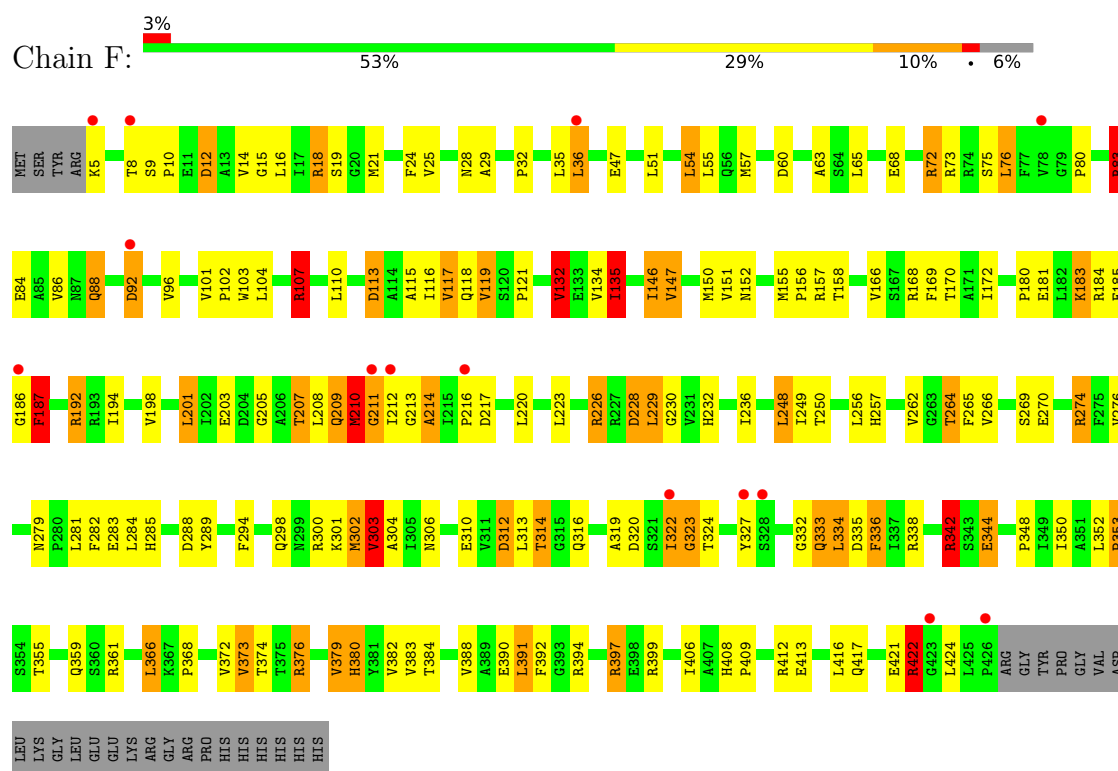
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	13	Total 13	O 13	0	0
2	C	13	Total 13	O 13	0	0
2	D	7	Total 7	O 7	0	0
2	E	8	Total 8	O 8	0	0
2	G	3	Total 3	O 3	0	0

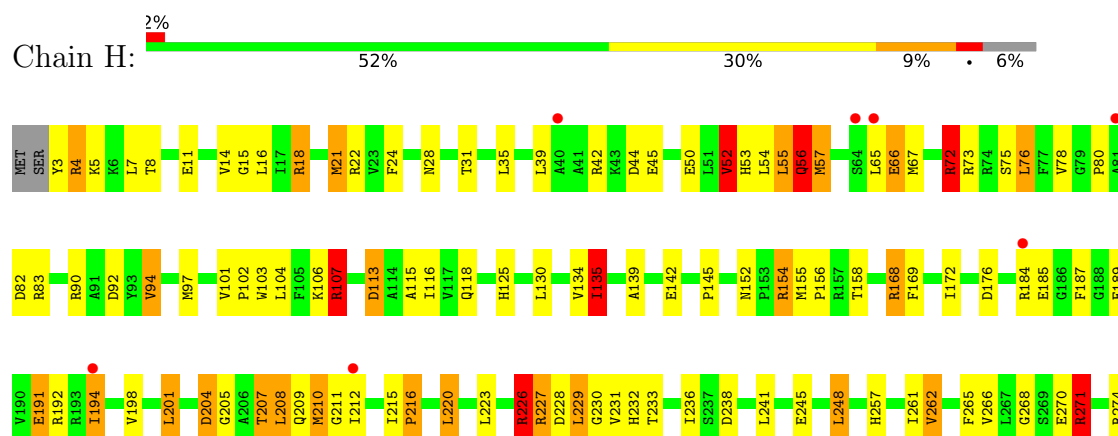
3 Residue-property plots [i](#)

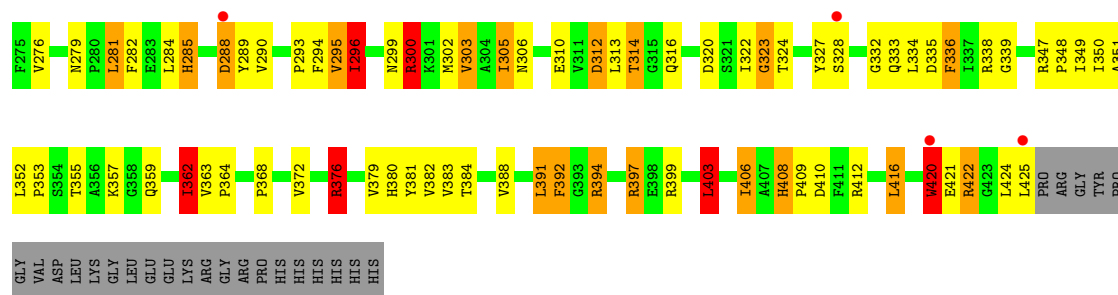
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 4-hydroxybutyrate coenzyme A transferase

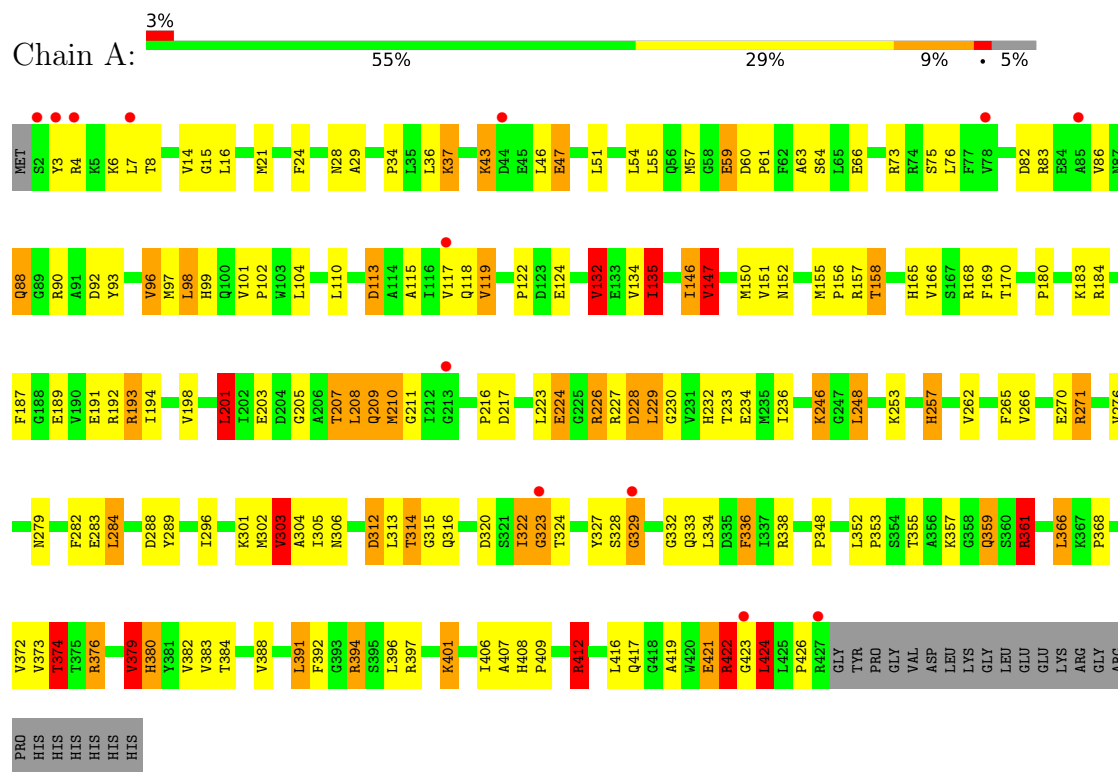


- Molecule 1: 4-hydroxybutyrate coenzyme A transferase

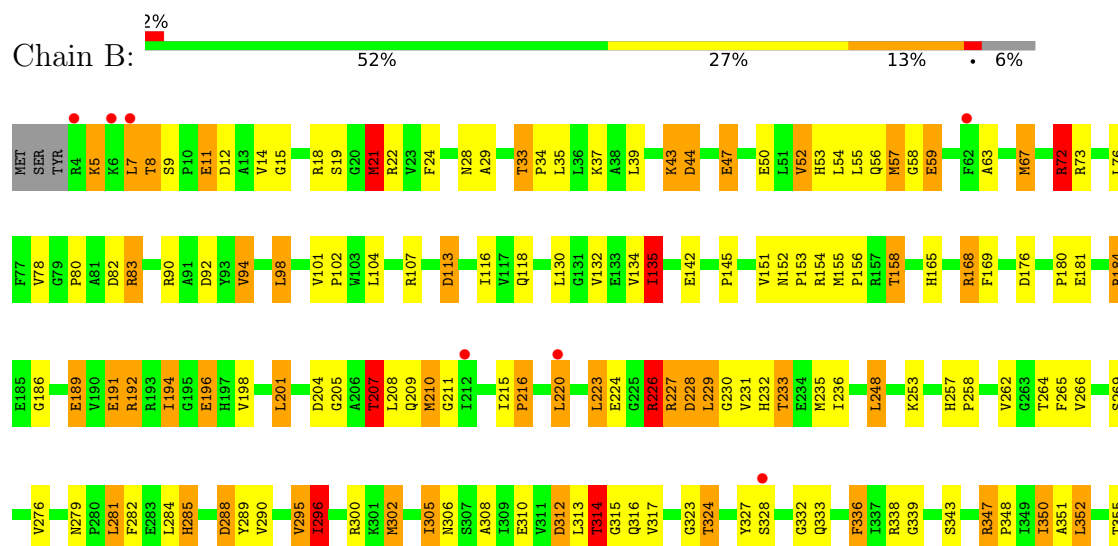


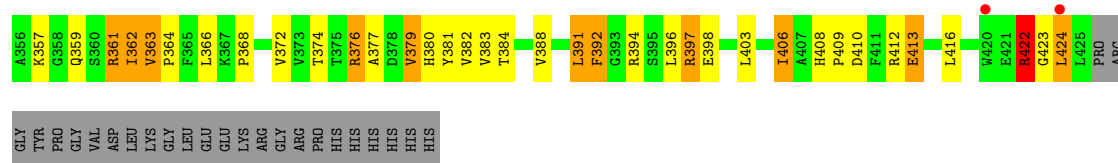


• Molecule 1: 4-hydroxybutyrate coenzyme A transferase

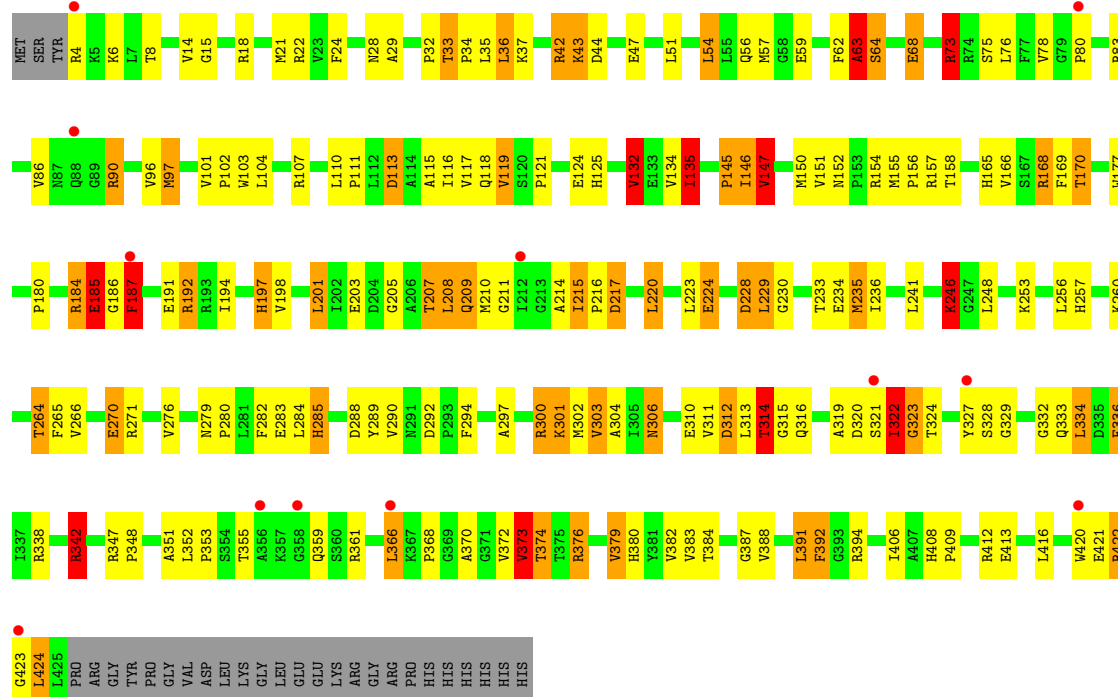


• Molecule 1: 4-hydroxybutyrate coenzyme A transferase

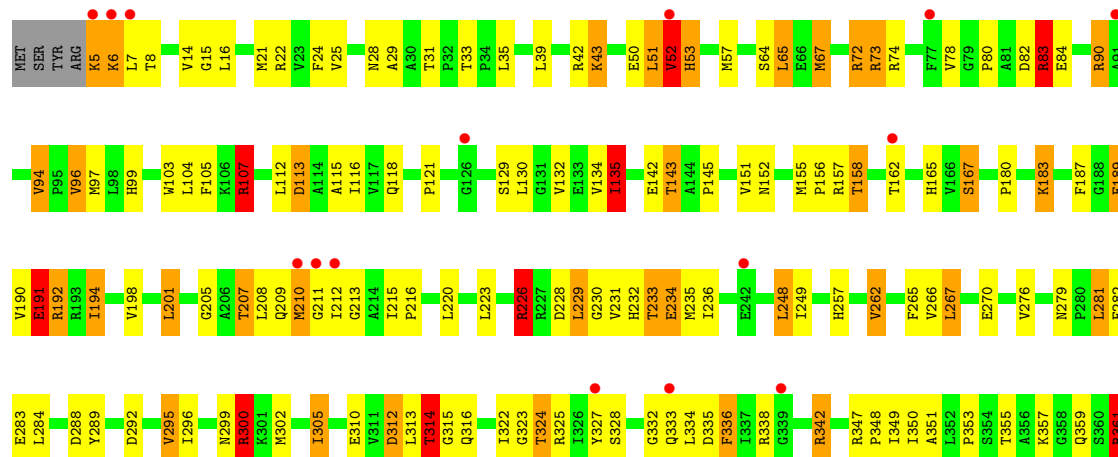


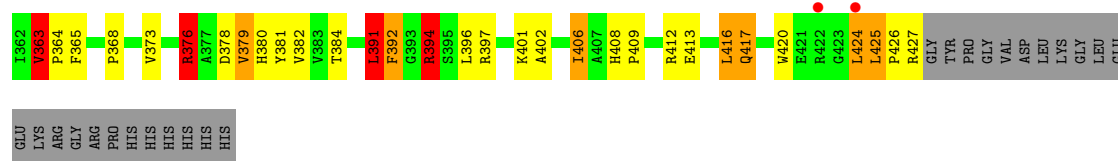


• Molecule 1: 4-hydroxybutyrate coenzyme A transferase

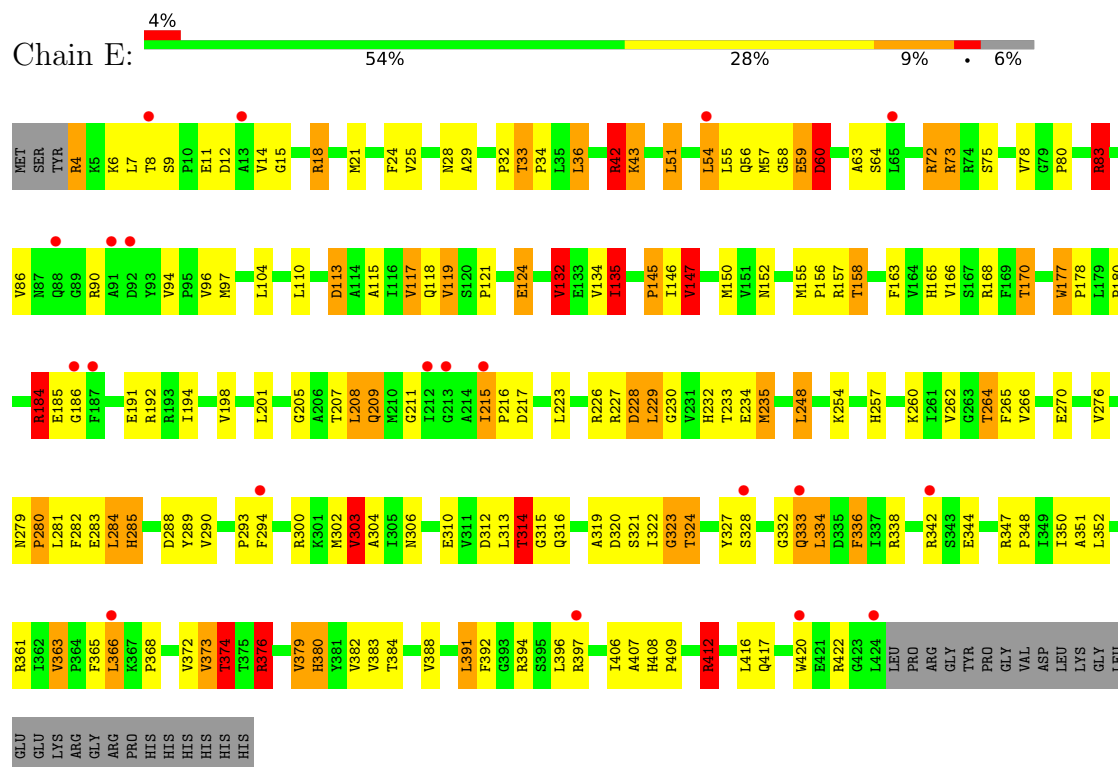


• Molecule 1: 4-hydroxybutyrate coenzyme A transferase

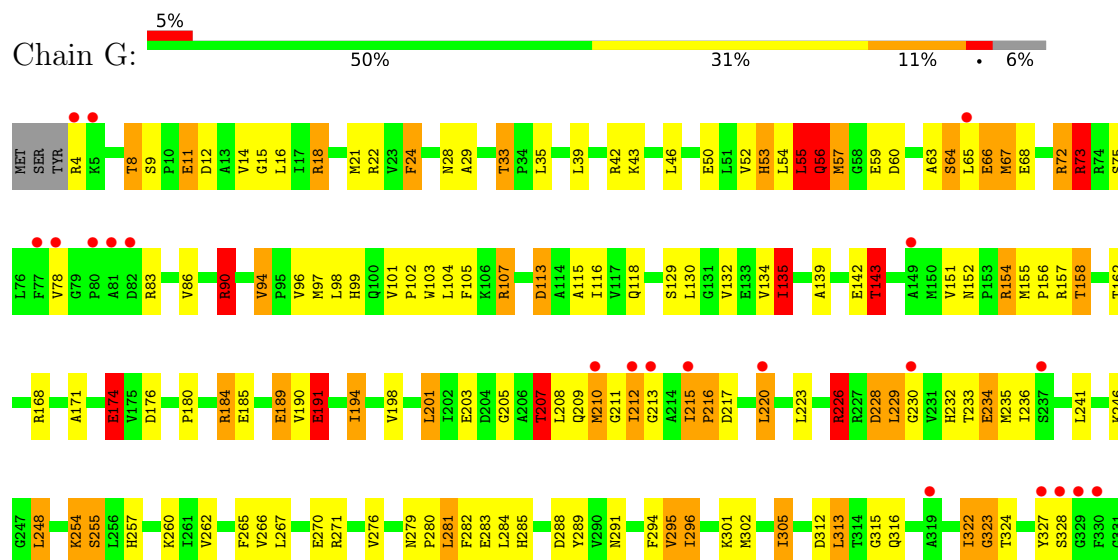


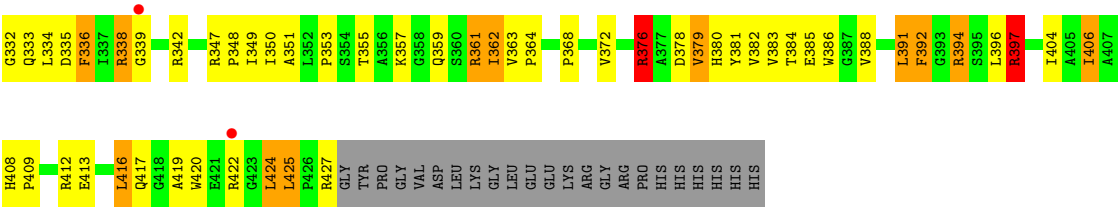


• Molecule 1: 4-hydroxybutyrate coenzyme A transferase



• Molecule 1: 4-hydroxybutyrate coenzyme A transferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	146.34Å 147.38Å 171.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.26 – 2.63 47.26 – 2.63	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.26-2.63) 97.4 (47.26-2.63)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.283 , 0.347 0.275 , 0.333	Depositor DCC
R_{free} test set	5326 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.41$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	25802	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7077e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.97	5/3348 (0.1%)	1.68	66/4547 (1.5%)
1	B	0.96	0/3265	1.66	52/4437 (1.2%)
1	C	0.96	2/3298 (0.1%)	1.72	69/4478 (1.5%)
1	D	0.97	2/3287 (0.1%)	1.67	59/4468 (1.3%)
1	E	0.97	0/3266	1.70	65/4439 (1.5%)
1	F	0.98	1/3286 (0.0%)	1.71	72/4465 (1.6%)
1	G	0.95	1/3281 (0.0%)	1.68	46/4461 (1.0%)
1	H	0.96	1/3275 (0.0%)	1.68	54/4452 (1.2%)
All	All	0.96	12/26306 (0.0%)	1.69	483/35747 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	9
1	C	0	12
1	D	0	12
1	E	0	12
1	F	0	6
1	G	0	12
1	H	0	11
All	All	0	82

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	322	ILE	C-O	-6.25	1.16	1.24
1	A	422	ARG	NE-CZ	5.94	1.39	1.33
1	F	312	ASP	CG-OD2	5.58	1.35	1.25
1	A	99	HIS	ND1-CE1	5.53	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	99	HIS	CG-CD2	-5.43	1.29	1.35
1	H	408	HIS	CD2-NE2	5.17	1.43	1.37
1	G	53	HIS	CD2-NE2	-5.13	1.32	1.37
1	A	257	HIS	CG-CD2	-5.13	1.30	1.35
1	C	311	VAL	C-O	-5.12	1.18	1.24
1	A	96	VAL	C-O	5.06	1.29	1.24
1	D	373	VAL	C-O	-5.04	1.18	1.23
1	A	312	ASP	CG-OD2	5.03	1.34	1.25

All (483) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	97	MET	CG-SD-CE	13.98	131.67	100.90
1	C	42	ARG	NE-CZ-NH2	13.60	131.44	119.20
1	E	42	ARG	NE-CZ-NH1	-13.38	108.12	121.50
1	C	288	ASP	CA-CB-CG	12.58	125.18	112.60
1	F	288	ASP	CA-CB-CG	12.46	125.06	112.60
1	H	403	LEU	N-CA-CB	12.42	128.96	110.33
1	E	288	ASP	CA-CB-CG	11.99	124.59	112.60
1	A	97	MET	CG-SD-CE	11.74	126.74	100.90
1	F	413	GLU	N-CA-CB	-11.68	93.08	110.01
1	G	254	LYS	N-CA-C	11.36	123.66	111.28
1	D	314	THR	CA-CB-OG1	-11.23	92.75	109.60
1	C	187	PHE	CA-CB-CG	-11.00	102.80	113.80
1	B	288	ASP	CA-CB-CG	10.89	123.49	112.60
1	A	288	ASP	CA-CB-CG	10.71	123.31	112.60
1	C	42	ARG	NE-CZ-NH1	-10.39	111.11	121.50
1	B	314	THR	CA-CB-OG1	-10.36	94.07	109.60
1	G	376	ARG	N-CA-CB	-10.26	93.36	110.39
1	G	288	ASP	CA-CB-CG	10.11	122.71	112.60
1	D	288	ASP	CA-CB-CG	10.04	122.64	112.60
1	C	170	THR	CA-CB-OG1	-9.99	94.61	109.60
1	G	97	MET	CG-SD-CE	9.96	122.82	100.90
1	H	288	ASP	CA-CB-CG	9.96	122.56	112.60
1	C	288	ASP	N-CA-CB	-9.87	95.02	110.22
1	A	424	LEU	N-CA-CB	-9.86	95.27	110.06
1	E	288	ASP	N-CA-CB	-9.81	95.11	110.22
1	E	42	ARG	NE-CZ-NH2	9.75	127.98	119.20
1	D	233	THR	CA-CB-OG1	-9.49	95.36	109.60
1	F	288	ASP	N-CA-CB	-9.48	95.62	110.22
1	H	288	ASP	N-CA-CB	-9.43	95.69	110.22
1	E	170	THR	CA-CB-OG1	-9.36	95.56	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	336	PHE	CA-CB-CG	-9.29	104.51	113.80
1	B	82	ASP	CA-CB-CG	9.17	121.77	112.60
1	C	424	LEU	N-CA-CB	9.15	125.95	110.49
1	A	288	ASP	N-CA-CB	-9.09	96.22	110.22
1	G	226	ARG	CG-CD-NE	-9.07	92.05	112.00
1	A	271	ARG	CB-CG-CD	9.04	132.08	111.30
1	H	191	GLU	CB-CG-CD	9.03	127.94	112.60
1	G	288	ASP	N-CA-CB	-8.93	96.47	110.22
1	B	5	LYS	CB-CA-C	8.91	125.48	111.13
1	B	336	PHE	CA-CB-CG	-8.80	105.00	113.80
1	G	189	GLU	CB-CG-CD	8.73	127.44	112.60
1	B	191	GLU	CB-CG-CD	8.68	127.36	112.60
1	D	336	PHE	CA-CB-CG	-8.55	105.25	113.80
1	H	336	PHE	CA-CB-CG	-8.52	105.28	113.80
1	H	362	ILE	CB-CA-C	8.51	122.85	110.77
1	C	374	THR	CA-CB-OG1	-8.50	96.85	109.60
1	C	246	LYS	CB-CG-CD	8.48	130.80	111.30
1	F	336	PHE	CA-CB-CG	-8.46	105.34	113.80
1	E	124	GLU	CB-CA-C	8.39	127.29	110.17
1	A	336	PHE	CA-CB-CG	-8.39	105.41	113.80
1	D	376	ARG	NE-CZ-NH1	-8.35	113.16	121.50
1	E	374	THR	CA-CB-OG1	-8.32	97.11	109.60
1	B	324	THR	CA-CB-OG1	8.27	122.01	109.60
1	D	97	MET	CG-SD-CE	8.27	119.09	100.90
1	G	174	GLU	N-CA-CB	8.22	124.38	110.49
1	D	210	MET	CG-SD-CE	-8.18	82.92	100.90
1	E	336	PHE	CA-CB-CG	-8.14	105.66	113.80
1	C	132	VAL	N-CA-CB	-8.10	93.67	111.81
1	B	288	ASP	N-CA-CB	-8.08	97.37	110.14
1	G	210	MET	CG-SD-CE	-8.07	83.14	100.90
1	F	117	VAL	N-CA-CB	-8.07	98.22	111.45
1	A	394	ARG	CG-CD-NE	-8.01	94.38	112.00
1	E	412	ARG	CG-CD-NE	7.98	129.55	112.00
1	E	132	VAL	N-CA-CB	-7.97	93.96	111.81
1	A	132	VAL	N-CA-CB	-7.91	94.10	111.81
1	C	270	GLU	CB-CG-CD	-7.89	99.19	112.60
1	G	191	GLU	CB-CG-CD	7.81	125.88	112.60
1	F	413	GLU	CB-CG-CD	-7.75	99.42	112.60
1	H	422	ARG	N-CA-CB	-7.74	98.60	110.44
1	F	132	VAL	N-CA-CB	-7.72	94.51	111.81
1	E	412	ARG	CD-NE-CZ	7.71	135.20	124.40
1	G	207	THR	CA-CB-OG1	7.67	121.11	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	264	THR	N-CA-CB	-7.64	100.84	111.00
1	E	422	ARG	CB-CA-C	-7.64	94.04	111.83
1	B	207	THR	CA-CB-OG1	7.60	121.01	109.60
1	C	312	ASP	CA-CB-CG	7.60	120.20	112.60
1	G	254	LYS	CA-C-O	-7.58	112.51	120.55
1	F	312	ASP	CA-CB-CG	7.58	120.18	112.60
1	F	302	MET	CG-SD-CE	7.55	117.52	100.90
1	D	376	ARG	NE-CZ-NH2	7.55	125.99	119.20
1	A	412	ARG	CG-CD-NE	7.52	128.55	112.00
1	D	6	LYS	N-CA-CB	-7.45	99.14	111.74
1	C	336	PHE	CA-CB-CG	-7.44	106.36	113.80
1	C	73	ARG	NE-CZ-NH2	7.42	125.88	119.20
1	F	5	LYS	CB-CA-C	7.40	124.15	110.10
1	H	420	TRP	N-CA-CB	7.40	122.46	110.40
1	G	72	ARG	CA-CB-CG	7.38	128.86	114.10
1	E	264	THR	N-CA-CB	-7.37	101.10	110.90
1	A	312	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	374	THR	CA-CB-OG1	-7.32	98.61	109.60
1	B	189	GLU	CB-CG-CD	7.30	125.01	112.60
1	F	187	PHE	N-CA-CB	7.29	122.81	110.49
1	E	60	ASP	N-CA-CB	7.29	123.34	110.37
1	F	394	ARG	CG-CD-NE	-7.26	96.03	112.00
1	B	312	ASP	CA-CB-CG	7.25	119.85	112.60
1	A	209	GLN	CG-CD-NE2	-7.20	105.61	116.40
1	E	184	ARG	CA-CB-CG	7.20	128.49	114.10
1	A	392	PHE	CB-CA-C	7.18	120.50	110.16
1	F	368	PRO	CB-CA-C	7.17	120.70	111.46
1	G	424	LEU	N-CA-CB	-7.16	99.47	110.92
1	B	392	PHE	CB-CA-C	7.15	120.45	110.16
1	G	397	ARG	CG-CD-NE	-7.15	96.28	112.00
1	C	285	HIS	O-C-N	-7.14	117.14	121.71
1	E	392	PHE	CB-CA-C	7.14	120.44	110.16
1	D	33	THR	CA-CB-OG1	-7.12	98.91	109.60
1	H	312	ASP	CA-CB-CG	7.10	119.70	112.60
1	H	56	GLN	N-CA-CB	7.08	122.46	110.49
1	H	420	TRP	CA-CB-CG	7.08	127.05	113.60
1	A	412	ARG	CD-NE-CZ	7.08	134.31	124.40
1	A	422	ARG	CG-CD-NE	7.08	127.56	112.00
1	D	324	THR	CA-CB-OG1	7.07	120.20	109.60
1	B	226	ARG	CA-CB-CG	-7.05	99.99	114.10
1	C	376	ARG	NE-CZ-NH2	7.05	125.55	119.20
1	E	124	GLU	CB-CG-CD	-7.05	100.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	422	ARG	CG-CD-NE	7.04	127.50	112.00
1	G	217	ASP	CA-CB-CG	7.03	119.63	112.60
1	B	285	HIS	O-C-N	-7.03	117.21	121.71
1	B	302	MET	CG-SD-CE	7.02	116.34	100.90
1	E	42	ARG	CD-NE-CZ	7.01	134.21	124.40
1	F	226	ARG	CB-CA-C	7.00	122.31	109.71
1	F	209	GLN	CG-CD-NE2	-6.99	105.92	116.40
1	H	392	PHE	CB-CA-C	6.98	120.79	109.90
1	F	121	PRO	N-CA-CB	6.97	107.09	103.19
1	C	394	ARG	CG-CD-NE	-6.96	96.69	112.00
1	F	392	PHE	CB-CA-C	6.95	120.17	110.16
1	G	174	GLU	CB-CG-CD	6.92	124.36	112.60
1	E	285	HIS	O-C-N	-6.89	117.30	121.71
1	C	42	ARG	CD-NE-CZ	6.87	134.02	124.40
1	G	285	HIS	O-C-N	-6.87	117.31	121.71
1	C	209	GLN	CG-CD-NE2	-6.86	106.11	116.40
1	D	72	ARG	CA-CB-CG	6.85	127.81	114.10
1	E	312	ASP	CA-CB-CG	6.83	119.44	112.60
1	C	228	ASP	CA-CB-CG	6.82	119.42	112.60
1	E	209	GLN	CG-CD-NE2	-6.82	106.17	116.40
1	H	210	MET	CG-SD-CE	-6.82	85.91	100.90
1	D	73	ARG	CD-NE-CZ	6.82	133.94	124.40
1	E	33	THR	CA-CB-OG1	-6.81	99.38	109.60
1	E	117	VAL	N-CA-CB	-6.80	99.19	111.92
1	C	342	ARG	CA-CB-CG	6.80	127.70	114.10
1	D	191	GLU	CB-CG-CD	6.77	124.11	112.60
1	A	147	VAL	N-CA-CB	6.76	122.38	111.23
1	D	143	THR	CA-CB-OG1	-6.73	99.50	109.60
1	F	207	THR	CA-CB-OG1	-6.73	99.51	109.60
1	F	226	ARG	N-CA-CB	-6.72	100.50	110.85
1	G	4	ARG	CB-CA-C	6.70	122.83	110.10
1	B	113	ASP	N-CA-C	-6.70	105.64	113.88
1	D	363	VAL	CB-CA-C	6.70	115.89	109.33
1	C	264	THR	CB-CA-C	6.66	119.53	109.13
1	F	92	ASP	CA-CB-CG	-6.66	105.94	112.60
1	G	226	ARG	CB-CG-CD	6.66	126.61	111.30
1	A	329	GLY	CA-C-O	-6.65	115.81	121.66
1	H	376	ARG	NE-CZ-NH2	6.64	125.18	119.20
1	D	361	ARG	NE-CZ-NH1	-6.64	114.86	121.50
1	F	342	ARG	CG-CD-NE	-6.64	97.39	112.00
1	E	376	ARG	NE-CZ-NH2	6.62	125.16	119.20
1	A	314	THR	CA-CB-OG1	-6.61	99.69	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	PHE	CA-CB-CG	6.60	120.40	113.80
1	C	392	PHE	CB-CA-C	6.59	120.18	109.90
1	C	300	ARG	CA-CB-CG	6.57	127.23	114.10
1	B	33	THR	CA-CB-OG1	-6.56	99.76	109.60
1	A	82	ASP	CA-CB-CG	6.54	119.14	112.60
1	F	422	ARG	NE-CZ-NH2	6.54	125.08	119.20
1	E	394	ARG	CG-CD-NE	-6.52	97.66	112.00
1	D	53	HIS	N-CA-C	6.52	124.68	110.80
1	D	72	ARG	N-CA-CB	-6.51	99.74	110.68
1	E	165	HIS	CA-CB-CG	-6.50	107.30	113.80
1	G	234	GLU	N-CA-CB	-6.49	100.01	110.14
1	E	228	ASP	CA-CB-CG	6.48	119.08	112.60
1	F	250	THR	N-CA-C	-6.47	106.60	114.75
1	A	117	VAL	N-CA-CB	-6.46	99.98	111.93
1	A	376	ARG	NE-CZ-NH1	-6.46	115.04	121.50
1	G	42	ARG	NE-CZ-NH1	6.43	127.93	121.50
1	A	73	ARG	CG-CD-NE	-6.42	97.87	112.00
1	A	376	ARG	CD-NE-CZ	-6.42	115.42	124.40
1	D	107	ARG	CG-CD-NE	6.41	126.10	112.00
1	F	264	THR	OG1-CB-CG2	6.40	122.09	109.30
1	G	33	THR	CA-CB-OG1	-6.40	100.01	109.60
1	B	210	MET	CG-SD-CE	-6.38	86.86	100.90
1	D	226	ARG	CB-CG-CD	-6.38	96.63	111.30
1	C	184	ARG	NE-CZ-NH2	6.37	124.94	119.20
1	G	338	ARG	CD-NE-CZ	6.37	133.31	124.40
1	A	92	ASP	CA-CB-CG	-6.36	106.24	112.60
1	A	124[A]	GLU	CB-CG-CD	6.36	123.40	112.60
1	A	124[B]	GLU	CB-CG-CD	6.36	123.40	112.60
1	F	320	ASP	CA-CB-CG	6.35	118.95	112.60
1	C	207	THR	CA-CB-OG1	-6.35	100.08	109.60
1	H	113	ASP	N-CA-C	-6.34	106.08	113.88
1	E	264	THR	CB-CA-C	6.34	119.67	109.02
1	F	390	GLU	CG-CD-OE2	-6.34	103.83	118.40
1	D	234	GLU	N-CA-CB	-6.33	100.27	110.14
1	E	4	ARG	CB-CA-C	6.32	122.12	110.10
1	A	37	LYS	CB-CG-CD	6.31	125.82	111.30
1	C	191	GLU	CB-CG-CD	6.31	123.33	112.60
1	E	113	ASP	N-CA-C	-6.31	106.12	113.88
1	C	33	THR	CA-CB-OG1	6.31	119.06	109.60
1	H	285	HIS	O-C-N	-6.30	117.68	121.71
1	H	295	VAL	N-CA-CB	6.30	121.08	110.56
1	B	43	LYS	CB-CG-CD	6.30	125.79	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	72	ARG	N-CA-CB	-6.30	100.88	110.77
1	C	113	ASP	N-CA-C	-6.28	105.93	113.97
1	F	264	THR	N-CA-CB	-6.27	102.66	111.00
1	H	158	THR	CA-CB-OG1	-6.26	100.20	109.60
1	B	223	LEU	N-CA-CB	-6.26	100.88	111.27
1	F	12	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	246	LYS	CB-CG-CD	6.25	125.67	111.30
1	F	88	GLN	CB-CA-C	-6.24	99.08	110.63
1	E	323	GLY	CA-C-N	6.22	128.91	120.38
1	E	323	GLY	C-N-CA	6.22	128.91	120.38
1	G	295	VAL	N-CA-CB	6.22	120.95	110.56
1	D	94	VAL	CA-C-O	6.21	123.61	119.38
1	C	314	THR	CA-CB-OG1	-6.21	100.29	109.60
1	H	28	ASN	CB-CA-C	6.21	122.77	110.42
1	D	424	LEU	N-CA-CB	-6.21	100.99	110.92
1	F	113	ASP	N-CA-C	-6.20	106.26	113.88
1	D	361	ARG	CB-CG-CD	6.19	125.54	111.30
1	D	73	ARG	CG-CD-NE	6.19	125.61	112.00
1	A	361	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	D	295	VAL	N-CA-CB	6.15	121.78	110.40
1	G	265	PHE	CA-CB-CG	6.15	119.95	113.80
1	A	380	HIS	CB-CG-ND1	6.14	131.91	122.70
1	B	310	GLU	N-CA-CB	-6.14	100.64	111.39
1	C	423	GLY	CA-C-N	6.13	133.26	121.54
1	C	423	GLY	C-N-CA	6.13	133.26	121.54
1	E	119	VAL	N-CA-CB	-6.13	100.85	110.96
1	F	5	LYS	N-CA-CB	-6.13	100.08	110.50
1	H	45	GLU	CB-CG-CD	-6.12	102.20	112.60
1	D	28	ASN	CB-CA-C	6.12	122.59	110.42
1	C	368	PRO	CB-CA-C	6.08	119.31	111.46
1	E	368	PRO	CB-CA-C	6.08	119.31	111.46
1	F	265	PHE	CA-CB-CG	6.08	119.88	113.80
1	E	170	THR	OG1-CB-CG2	-6.07	97.15	109.30
1	F	333	GLN	OE1-CD-NE2	6.07	128.66	122.60
1	H	368	PRO	CB-CA-C	6.06	119.27	111.21
1	A	113	ASP	N-CA-C	-6.06	106.43	113.88
1	H	52	VAL	N-CA-CB	6.04	118.24	110.99
1	H	154	ARG	CB-CG-CD	6.04	125.19	111.30
1	E	121	PRO	N-CA-CB	6.03	106.57	103.19
1	B	158	THR	CA-CB-OG1	-6.01	100.59	109.60
1	H	226	ARG	CB-CG-CD	6.00	125.10	111.30
1	E	264	THR	CA-CB-OG1	-6.00	100.60	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	28	ASN	CB-CA-C	5.99	122.35	110.42
1	C	119	VAL	N-CA-CB	-5.99	99.72	112.00
1	B	235	MET	CG-SD-CE	5.99	114.08	100.90
1	A	193	ARG	CD-NE-CZ	5.97	132.76	124.40
1	G	113	ASP	N-CA-C	-5.97	106.53	113.88
1	D	310	GLU	N-CA-CB	-5.97	100.94	111.39
1	C	86	VAL	N-CA-CB	5.96	121.56	110.77
1	H	57	MET	CG-SD-CE	5.96	114.01	100.90
1	A	226	ARG	N-CA-CB	-5.96	101.68	110.85
1	B	352	LEU	CB-CG-CD1	5.95	128.56	110.70
1	B	363	VAL	N-CA-CB	-5.95	105.27	111.64
1	F	86	VAL	N-CA-CB	5.95	121.53	110.77
1	F	264	THR	CB-CA-C	5.93	118.39	109.13
1	B	72	ARG	CB-CG-CD	5.93	124.94	111.30
1	A	379	VAL	N-CA-CB	5.93	118.38	110.26
1	A	119	VAL	N-CA-CB	-5.92	99.86	112.00
1	E	422	ARG	N-CA-C	5.92	117.64	109.54
1	B	107	ARG	CG-CD-NE	5.91	125.00	112.00
1	E	28	ASN	CB-CA-C	5.90	122.15	110.42
1	G	228	ASP	CA-CB-CG	5.89	118.49	112.60
1	F	274	ARG	CA-CB-CG	5.89	125.89	114.10
1	E	191	GLU	CB-CG-CD	5.89	122.61	112.60
1	A	28	ASN	CB-CA-C	5.88	122.12	110.42
1	B	368	PRO	CB-CA-C	5.88	119.05	111.46
1	G	338	ARG	CG-CD-NE	5.88	124.94	112.00
1	B	28	ASN	CB-CA-C	5.88	122.12	110.42
1	E	145	PRO	CB-CA-C	5.88	121.38	112.21
1	H	4	ARG	N-CA-CB	-5.87	100.57	110.49
1	F	228	ASP	CA-CB-CG	5.86	118.46	112.60
1	H	422	ARG	CB-CA-C	5.85	120.54	110.01
1	C	264	THR	OG1-CB-CG2	5.85	121.00	109.30
1	H	82	ASP	CA-CB-CG	5.84	118.44	112.60
1	F	379	VAL	N-CA-CB	5.84	120.71	110.49
1	C	342	ARG	N-CA-CB	5.83	119.11	110.53
1	D	158	THR	CA-CB-OG1	-5.83	100.86	109.60
1	F	185	GLU	CB-CG-CD	-5.82	102.70	112.60
1	D	392	PHE	CB-CA-C	5.82	118.54	110.16
1	F	158	THR	CA-CB-OG1	-5.82	100.88	109.60
1	C	68	GLU	CG-CD-OE1	-5.81	105.04	118.40
1	B	72	ARG	CB-CA-C	5.81	120.34	109.71
1	D	99	HIS	CA-CB-CG	5.81	119.61	113.80
1	E	117	VAL	CA-CB-CG1	5.81	120.27	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	125	HIS	CA-CB-CG	-5.81	107.99	113.80
1	F	379	VAL	CB-CA-C	-5.80	103.63	111.63
1	D	406	ILE	N-CA-CB	-5.80	103.26	112.07
1	H	169	PHE	CB-CA-C	-5.79	99.76	109.48
1	A	86	VAL	N-CA-CB	5.79	121.24	110.77
1	A	184	ARG	CG-CD-NE	-5.77	99.30	112.00
1	A	226	ARG	CB-CA-C	5.76	120.08	109.71
1	E	300	ARG	CA-CB-CG	5.75	125.61	114.10
1	C	158	THR	CA-CB-OG1	-5.75	100.97	109.60
1	G	99	HIS	CA-CB-CG	5.75	119.55	113.80
1	C	300	ARG	CB-CA-C	5.74	120.03	109.46
1	F	187	PHE	CA-CB-CG	5.74	119.54	113.80
1	A	265	PHE	CA-CB-CG	5.74	119.54	113.80
1	C	43	LYS	CA-CB-CG	5.74	125.57	114.10
1	G	28	ASN	CB-CA-C	5.73	121.83	110.42
1	F	117	VAL	CA-CB-CG1	5.73	120.14	110.40
1	A	314	THR	CA-C-N	-5.73	116.66	123.08
1	A	314	THR	C-N-CA	-5.73	116.66	123.08
1	E	363	VAL	CB-CA-C	5.71	114.93	109.33
1	H	45	GLU	N-CA-CB	5.71	119.57	110.73
1	D	312	ASP	CA-CB-CG	5.70	118.30	112.60
1	D	361	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	158	THR	CA-CB-OG1	-5.70	101.06	109.60
1	D	121	PRO	N-CA-CB	5.69	106.38	103.19
1	E	184	ARG	CG-CD-NE	5.69	124.52	112.00
1	C	320	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	373	VAL	CA-C-N	-5.67	114.99	122.99
1	C	373	VAL	C-N-CA	-5.67	114.99	122.99
1	G	392	PHE	CB-CA-C	5.67	118.75	109.90
1	G	234	GLU	CB-CG-CD	-5.67	102.96	112.60
1	A	424	LEU	N-CA-C	5.66	118.18	111.33
1	F	421	GLU	CB-CG-CD	5.66	122.21	112.60
1	F	211	GLY	CA-C-N	-5.65	114.92	122.77
1	F	211	GLY	C-N-CA	-5.65	114.92	122.77
1	F	285	HIS	O-C-N	-5.65	118.09	121.71
1	A	303	VAL	N-CA-CB	5.65	119.02	111.90
1	A	368	PRO	CB-CA-C	5.65	118.75	111.46
1	E	72	ARG	N-CA-CB	-5.64	101.21	110.68
1	C	264	THR	CA-CB-OG1	-5.63	101.16	109.60
1	E	43	LYS	CA-CB-CG	5.62	125.34	114.10
1	H	52	VAL	CB-CA-C	-5.62	103.20	110.84
1	H	310	GLU	N-CA-CB	-5.62	101.56	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	PRO	N-CA-CB	5.61	106.33	103.19
1	B	295	VAL	N-CA-CB	5.61	120.78	110.40
1	E	376	ARG	CB-CG-CD	5.61	124.21	111.30
1	G	335	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	228	ASP	CA-CB-CG	5.60	118.20	112.60
1	C	165	HIS	CA-CB-CG	-5.60	108.20	113.80
1	F	73	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	H	262	VAL	N-CA-CB	-5.60	104.62	110.72
1	B	226	ARG	CG-CD-NE	5.59	124.31	112.00
1	E	147	VAL	N-CA-CB	5.59	120.46	111.23
1	D	42	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	G	73	ARG	CG-CD-NE	5.58	124.29	112.00
1	A	201	LEU	N-CA-C	-5.58	106.82	113.97
1	E	380	HIS	CB-CG-ND1	5.58	131.08	122.70
1	E	280	PRO	CB-CA-C	-5.57	103.49	111.62
1	H	271	ARG	CA-CB-CG	5.56	125.22	114.10
1	H	66	GLU	N-CA-CB	5.55	120.42	110.32
1	C	270	GLU	CG-CD-OE2	-5.54	105.65	118.40
1	C	44	ASP	CA-CB-CG	5.54	118.14	112.60
1	D	376	ARG	CB-CG-CD	5.54	124.03	111.30
1	C	310	GLU	CB-CG-CD	5.53	122.00	112.60
1	F	73	ARG	CG-CD-NE	-5.53	99.84	112.00
1	H	376	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	C	145	PRO	CB-CA-C	5.52	120.82	112.21
1	C	57	MET	CG-SD-CE	5.51	113.03	100.90
1	D	368	PRO	CB-CA-C	5.50	118.56	111.46
1	A	423	GLY	CA-C-N	5.50	127.92	120.38
1	A	423	GLY	C-N-CA	5.50	127.92	120.38
1	C	310	GLU	CB-CA-C	5.50	120.23	110.16
1	A	228	ASP	CA-CB-CG	5.50	118.10	112.60
1	H	335	ASP	CA-CB-CG	5.50	118.09	112.60
1	D	6	LYS	N-CA-C	5.49	116.88	107.28
1	F	210	MET	CG-SD-CE	-5.48	88.84	100.90
1	C	33	THR	OG1-CB-CG2	-5.48	98.33	109.30
1	G	158	THR	CA-CB-OG1	-5.48	101.39	109.60
1	F	119	VAL	N-CA-CB	-5.46	100.80	112.00
1	D	265	PHE	CA-CB-CG	5.46	119.26	113.80
1	H	21	MET	CB-CA-C	5.45	118.74	109.53
1	H	107	ARG	CG-CD-NE	5.45	123.98	112.00
1	C	197	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	D	425	LEU	CB-CA-C	-5.45	99.44	110.17
1	D	52	VAL	O-C-N	-5.43	115.78	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	HIS	CA-CB-CG	-5.43	108.37	113.80
1	H	300	ARG	CB-CA-C	5.42	119.44	109.46
1	D	425	LEU	N-CA-CB	5.42	120.02	110.37
1	A	43	LYS	CA-CB-CG	5.42	124.93	114.10
1	G	368	PRO	CB-CA-C	5.42	118.45	111.46
1	D	113	ASP	N-CA-C	-5.40	107.24	113.88
1	C	342	ARG	CB-CA-C	5.39	119.10	109.29
1	G	56	GLN	N-CA-CB	5.39	119.60	110.49
1	D	82	ASP	CA-CB-CG	5.39	117.99	112.60
1	H	72	ARG	CB-CA-C	5.39	119.45	109.70
1	A	271	ARG	CG-CD-NE	5.39	123.85	112.00
1	H	420	TRP	CB-CA-C	5.38	121.24	109.99
1	B	363	VAL	CB-CA-C	5.38	114.61	109.33
1	C	147	VAL	N-CA-CB	5.38	120.11	111.23
1	F	72	ARG	N-CA-CB	-5.37	101.65	110.68
1	A	328	SER	CA-CB-OG	5.37	121.83	111.10
1	B	21	MET	CB-CA-C	5.37	118.60	109.53
1	G	413	GLU	N-CA-CB	5.37	117.79	110.01
1	A	271	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	H	231	VAL	N-CA-C	5.34	115.65	108.17
1	H	353	PRO	CB-CA-C	5.34	118.06	111.23
1	F	380	HIS	CB-CG-ND1	5.34	130.71	122.70
1	F	303	VAL	N-CA-CB	5.32	118.60	111.90
1	C	125	HIS	CA-CB-CG	-5.31	108.49	113.80
1	H	296	ILE	CA-CB-CG2	5.31	119.52	110.50
1	D	394	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	D	335	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	421	GLU	CA-C-O	-5.29	114.94	120.55
1	B	296	ILE	CA-CB-CG2	5.29	119.49	110.50
1	F	214	ALA	CA-C-N	5.28	124.56	120.33
1	F	214	ALA	C-N-CA	5.28	124.56	120.33
1	F	76	LEU	CB-CG-CD1	-5.28	94.87	110.70
1	F	413	GLU	CB-CA-C	-5.27	102.60	110.88
1	B	72	ARG	CD-NE-CZ	5.27	131.78	124.40
1	D	233	THR	CA-CB-CG2	5.27	119.45	110.50
1	E	303	VAL	N-CA-CB	5.26	118.53	111.90
1	F	421	GLU	CG-CD-OE2	-5.26	106.31	118.40
1	H	265	PHE	CA-CB-CG	5.26	119.06	113.80
1	E	86	VAL	N-CA-CB	5.25	120.27	110.77
1	E	314	THR	CA-CB-OG1	5.25	117.47	109.60
1	H	204	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	184	ARG	CG-CD-NE	5.24	123.52	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	GLU	CB-CG-CD	5.23	121.50	112.60
1	D	96	VAL	N-CA-CB	-5.23	103.11	111.58
1	H	320	ASP	CA-CB-CG	5.22	117.82	112.60
1	C	117	VAL	N-CA-CB	-5.22	102.16	111.92
1	E	380	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	B	422	ARG	NE-CZ-NH1	-5.21	116.28	121.50
1	C	265	PHE	CA-CB-CG	5.21	119.01	113.80
1	E	11	GLU	CB-CG-CD	5.20	121.45	112.60
1	F	380	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	E	324	THR	N-CA-CB	-5.20	102.26	110.06
1	F	310	GLU	CA-CB-CG	5.20	124.50	114.10
1	B	227	ARG	CA-CB-CG	5.20	124.50	114.10
1	F	264	THR	CA-CB-OG1	-5.19	101.81	109.60
1	B	231	VAL	N-CA-C	5.18	115.43	108.17
1	A	394	ARG	NH1-CZ-NH2	5.18	126.04	119.30
1	C	4	ARG	CB-CA-C	5.18	119.94	110.10
1	F	399	ARG	O-C-N	5.18	128.05	122.15
1	A	43	LYS	CB-CG-CD	-5.17	99.40	111.30
1	D	5	LYS	CB-CA-C	5.17	119.93	110.10
1	B	352	LEU	CB-CG-CD2	-5.17	95.19	110.70
1	D	72	ARG	CD-NE-CZ	5.17	131.63	124.40
1	G	24	PHE	CA-CB-CG	-5.16	108.64	113.80
1	F	300	ARG	CA-CB-CG	5.16	124.42	114.10
1	F	249	ILE	O-C-N	5.16	128.67	123.20
1	C	420	TRP	CB-CA-C	5.16	121.09	110.31
1	E	314	THR	CB-CA-C	-5.16	100.89	109.55
1	B	233	THR	CA-CB-CG2	5.16	119.26	110.50
1	C	185	GLU	N-CA-C	5.16	117.31	111.02
1	F	335	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	73	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	H	187	PHE	CA-CB-CG	5.15	118.95	113.80
1	A	357	LYS	N-CA-CB	5.15	119.87	110.60
1	B	264	THR	CA-CB-OG1	-5.15	101.88	109.60
1	B	165	HIS	CA-CB-CG	-5.14	108.66	113.80
1	A	314	THR	OG1-CB-CG2	5.14	119.58	109.30
1	A	320	ASP	CA-CB-CG	5.14	117.74	112.60
1	E	51	LEU	N-CA-CB	-5.14	101.50	109.87
1	B	169	PHE	CB-CA-C	-5.13	100.86	109.48
1	F	376	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	G	86	VAL	N-CA-CB	5.13	120.05	110.77
1	E	310	GLU	CB-CG-CD	5.12	121.31	112.60
1	H	21	MET	CG-SD-CE	5.12	112.16	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	177	TRP	CA-CB-CG	-5.11	103.89	113.60
1	B	374	THR	CA-CB-OG1	5.10	117.25	109.60
1	F	288	ASP	N-CA-C	-5.10	105.85	111.71
1	D	267	LEU	N-CA-CB	-5.10	102.25	110.81
1	H	376	ARG	CB-CG-CD	5.08	122.99	111.30
1	B	253	LYS	CA-CB-CG	-5.08	103.94	114.10
1	D	391	LEU	N-CA-CB	-5.08	103.06	110.47
1	G	143	THR	CA-CB-CG2	5.07	119.12	110.50
1	E	158	THR	CA-CB-OG1	-5.07	102.00	109.60
1	D	310	GLU	CA-CB-CG	5.06	124.22	114.10
1	A	380	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	D	262	VAL	N-CA-CB	-5.06	105.21	110.72
1	F	288	ASP	CB-CA-C	5.06	119.98	110.63
1	E	265	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	61	PRO	CB-CA-C	5.05	115.66	110.00
1	G	94	VAL	CA-C-O	5.05	122.81	119.38
1	E	90	ARG	CG-CD-NE	-5.05	100.89	112.00
1	E	320	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	73	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	C	306	ASN	CA-CB-CG	-5.04	107.56	112.60
1	D	231	VAL	N-CA-CB	-5.04	104.40	111.25
1	A	397	ARG	CB-CA-C	5.03	119.19	110.84
1	B	98	LEU	CB-CG-CD1	-5.03	95.61	110.70
1	H	422	ARG	CA-CB-CG	5.03	124.15	114.10
1	D	231	VAL	N-CA-C	5.03	115.21	108.17
1	B	52	VAL	N-CA-CB	5.02	118.90	110.86
1	F	353	PRO	CB-CA-C	5.01	117.65	111.23
1	C	97	MET	CG-SD-CE	5.01	111.92	100.90
1	A	253	LYS	CB-CG-CD	5.01	122.82	111.30
1	B	361	ARG	CA-C-N	-5.01	116.44	123.10
1	B	361	ARG	C-N-CA	-5.01	116.44	123.10
1	G	312	ASP	CA-CB-CG	5.00	117.61	112.60
1	C	28	ASN	CB-CA-C	5.00	120.37	110.42

There are no chirality outliers.

All (82) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ARG	Sidechain
1	A	193	ARG	Sidechain
1	A	227	ARG	Sidechain
1	A	361	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	394	ARG	Sidechain
1	A	4[A]	ARG	Sidechain
1	A	412	ARG	Sidechain
1	A	422	ARG	Sidechain
1	B	168	ARG	Sidechain
1	B	192	ARG	Sidechain
1	B	226	ARG	Sidechain
1	B	347	ARG	Sidechain
1	B	361	ARG	Sidechain
1	B	376	ARG	Sidechain
1	B	422	ARG	Sidechain
1	B	5	LYS	Peptide
1	B	58	GLY	Peptide
1	C	154	ARG	Sidechain
1	C	157	ARG	Sidechain
1	C	192	ARG	Sidechain
1	C	300	ARG	Sidechain
1	C	321	SER	Peptide
1	C	329	GLY	Peptide
1	C	347	ARG	Sidechain
1	C	42	ARG	Sidechain
1	C	422	ARG	Sidechain
1	C	63	ALA	Peptide
1	C	73	ARG	Sidechain
1	C	90	ARG	Sidechain
1	D	107	ARG	Sidechain
1	D	157	ARG	Sidechain
1	D	192	ARG	Sidechain
1	D	300	ARG	Sidechain
1	D	361	ARG	Sidechain
1	D	376	ARG	Sidechain
1	D	394	ARG	Sidechain
1	D	397	ARG	Sidechain
1	D	5	LYS	Peptide
1	D	73	ARG	Sidechain
1	D	83	ARG	Sidechain
1	D	90	ARG	Sidechain
1	E	157	ARG	Sidechain
1	E	18	ARG	Sidechain
1	E	184	ARG	Sidechain
1	E	186	GLY	Peptide
1	E	227	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	347	ARG	Sidechain
1	E	361	ARG	Sidechain
1	E	376	ARG	Sidechain
1	E	412	ARG	Sidechain
1	E	42	ARG	Sidechain
1	E	73	ARG	Sidechain
1	E	83	ARG	Sidechain
1	F	107	ARG	Sidechain
1	F	157	ARG	Sidechain
1	F	18	ARG	Sidechain
1	F	184	ARG	Sidechain
1	F	342	ARG	Sidechain
1	F	83	ARG	Sidechain
1	G	107	ARG	Sidechain
1	G	154	ARG	Sidechain
1	G	157	ARG	Sidechain
1	G	18	ARG	Sidechain
1	G	226	ARG	Sidechain
1	G	347	ARG	Sidechain
1	G	361	ARG	Sidechain
1	G	376	ARG	Sidechain
1	G	397	ARG	Sidechain
1	G	55	LEU	Mainchain
1	G	73	ARG	Sidechain
1	G	90	ARG	Sidechain
1	H	107	ARG	Sidechain
1	H	168	ARG	Sidechain
1	H	18	ARG	Sidechain
1	H	271	ARG	Sidechain
1	H	362	ILE	Peptide
1	H	376	ARG	Sidechain
1	H	397	ARG	Sidechain
1	H	42	ARG	Sidechain
1	H	72	ARG	Sidechain
1	H	73	ARG	Sidechain
1	H	90	ARG	Sidechain

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	3277	0	3288	99	0
1	B	3197	0	3198	126	0
1	C	3226	0	3238	122	0
1	D	3217	0	3232	115	0
1	E	3196	0	3187	114	0
1	F	3216	0	3234	123	0
1	G	3211	0	3214	141	0
1	H	3206	0	3210	123	0
2	A	11	0	0	1	0
2	B	13	0	0	3	0
2	C	13	0	0	1	0
2	D	7	0	0	1	0
2	E	8	0	0	1	0
2	G	3	0	0	0	0
2	H	1	0	0	0	0
All	All	25802	0	25801	907	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 18.

All (907) 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:G:139:ALA:O	1:G:143:THR:HG22	1.44	1.16
1:B:423:GLY:O	1:B:424:LEU:HG	1.47	1.12
1:A:333:GLN:HE21	1:A:374:THR:CG2	1.64	1.10
1:H:399:ARG:O	1:H:403:LEU:HD22	1.51	1.09
1:C:333:GLN:HE21	1:C:374:THR:CG2	1.66	1.08
1:C:338:ARG:NH2	1:D:334:LEU:HD21	1.70	1.06
1:C:323:GLY:HA2	1:C:370:ALA:HA	1.38	1.04
1:F:210:MET:HE1	1:F:220:LEU:HD21	1.41	1.03
1:D:31:THR:HG21	1:D:57:MET:O	1.55	1.03
1:B:209:GLN:HA	1:B:233:THR:HG22	1.42	1.02
1:C:333:GLN:HE21	1:C:374:THR:HG23	1.24	0.99
1:H:209:GLN:HA	1:H:233:THR:HG22	1.44	0.96
1:G:64:SER:H	1:G:90:ARG:HH11	1.11	0.95
1:B:364:PRO:O	1:B:422:ARG:NH1	2.00	0.93
1:H:410:ASP:OD2	1:G:420:TRP:NE1	2.01	0.93
1:A:209:GLN:HE22	1:A:306:ASN:HD21	1.16	0.92
1:C:319:ALA:HB3	1:C:373:VAL:HG11	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:GLN:HE22	1:E:306:ASN:HD21	1.14	0.91
1:A:333:GLN:HE21	1:A:374:THR:HG23	1.33	0.91
1:D:194:ILE:HD11	1:D:351:ALA:HB1	1.50	0.90
1:B:410:ASP:OD2	1:D:420:TRP:NE1	2.04	0.90
1:C:338:ARG:HH21	1:D:334:LEU:HD21	1.34	0.90
1:E:319:ALA:HB3	1:E:373:VAL:HG11	1.53	0.89
1:F:319:ALA:HB3	1:F:373:VAL:HG11	1.53	0.88
1:B:296:ILE:HG12	1:B:339:GLY:HA3	1.55	0.87
1:F:312:ASP:OD1	1:F:314:THR:HG22	1.74	0.87
1:A:37:LYS:NZ	1:A:59:GLU:OE1	2.07	0.87
1:H:208:LEU:HD12	1:H:303:VAL:HG13	1.56	0.86
1:B:312:ASP:OD1	1:B:314:THR:HG22	1.75	0.86
1:G:154:ARG:HD2	1:G:176:ASP:OD1	1.74	0.86
1:C:208:LEU:HD12	1:C:303:VAL:HG22	1.55	0.86
1:E:97:MET:HE1	1:G:378:ASP:OD1	1.76	0.85
1:F:397:ARG:HG3	1:H:92:ASP:OD1	1.76	0.85
1:C:62:PHE:O	1:C:64:SER:N	2.09	0.85
1:H:296:ILE:HG12	1:H:339:GLY:HA3	1.57	0.85
1:G:194:ILE:HD11	1:G:351:ALA:HB1	1.59	0.83
1:F:208:LEU:HD23	1:F:303:VAL:HG22	1.60	0.83
1:D:165:HIS:HD2	1:D:167:SER:HB2	1.44	0.83
1:G:296:ILE:HG12	1:G:339:GLY:HA3	1.61	0.83
1:F:209:GLN:HE22	1:F:306:ASN:HD21	1.21	0.82
1:H:314:THR:HG21	1:H:376:ARG:HH11	1.41	0.82
1:F:417:GLN:OE1	1:C:145:PRO:HG3	1.79	0.82
1:H:312:ASP:OD1	1:H:314:THR:HG22	1.78	0.82
1:E:208:LEU:HD12	1:E:303:VAL:HG22	1.62	0.81
1:E:314:THR:HG22	1:E:396:LEU:HD22	1.61	0.81
1:D:312:ASP:OD1	1:D:314:THR:HG22	1.80	0.81
1:F:103:TRP:HB3	1:F:107:ARG:HD2	1.62	0.81
1:G:212:ILE:HB	1:G:235:MET:SD	2.21	0.81
1:B:423:GLY:O	1:B:424:LEU:CG	2.27	0.81
1:C:314:THR:HG21	1:C:376:ARG:HH11	1.45	0.80
1:C:333:GLN:NE2	1:C:374:THR:HG23	1.95	0.80
1:C:33:THR:OG1	1:C:177:TRP:CZ2	2.33	0.80
1:C:103:TRP:HB3	1:C:107[A]:ARG:HD2	1.61	0.80
1:C:314:THR:HG21	1:C:376:ARG:NH1	1.97	0.79
1:H:54:LEU:O	1:H:55:LEU:O	2.01	0.79
1:H:399:ARG:O	1:H:403:LEU:CD2	2.30	0.79
1:A:384:THR:HG23	1:A:406:ILE:HD13	1.64	0.78
1:H:403:LEU:HD22	1:H:403:LEU:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ARG:O	1:B:168:ARG:NH1	2.17	0.78
1:E:333:GLN:NE2	1:E:374:THR:CG2	2.46	0.78
1:F:384:THR:HG23	1:F:406:ILE:HD13	1.65	0.78
1:D:314:THR:HG21	1:D:376:ARG:HH11	1.46	0.78
1:D:296:ILE:HG23	1:D:302:MET:HE3	1.66	0.78
1:E:184:ARG:NH2	1:E:217:ASP:OD2	2.15	0.78
1:F:210:MET:HE1	1:F:220:LEU:CD2	2.14	0.77
1:H:208:LEU:HD12	1:H:303:VAL:CG1	2.14	0.77
1:G:64:SER:N	1:G:90:ARG:HH11	1.83	0.77
1:C:323:GLY:HA2	1:C:370:ALA:CA	2.12	0.77
1:G:63:ALA:O	1:G:64:SER:HB2	1.85	0.76
1:C:56:GLN:HE21	1:C:73:ARG:HH12	1.34	0.76
1:F:256:LEU:HD13	1:F:298:GLN:HE21	1.50	0.76
1:F:32:PRO:CA	1:F:150:MET:HE1	2.16	0.75
1:G:139:ALA:O	1:G:143:THR:CG2	2.31	0.75
1:B:43:LYS:HB2	1:B:67:MET:HE3	1.68	0.75
1:A:208:LEU:HD12	1:A:303:VAL:HG22	1.68	0.75
1:C:209:GLN:HG2	1:C:336:PHE:CD1	2.21	0.75
1:F:209:GLN:HG2	1:F:336:PHE:CD1	2.21	0.74
1:D:349:ILE:HD13	1:D:381:TYR:HB2	1.68	0.74
1:A:333:GLN:NE2	1:A:374:THR:HG23	2.03	0.74
1:B:210:MET:HE1	1:B:220:LEU:HD13	1.70	0.73
1:A:209:GLN:HG2	1:A:336:PHE:CD1	2.22	0.73
1:F:80:PRO:HA	1:F:83:ARG:HH11	1.53	0.73
1:B:7:LEU:O	1:B:7:LEU:HD13	1.89	0.73
1:F:344:GLU:OE1	1:F:344:GLU:HA	1.89	0.73
1:G:232:HIS:HB3	1:G:302:MET:HE1	1.70	0.73
1:F:314:THR:HG21	1:F:376:ARG:HH11	1.53	0.73
1:D:165:HIS:CD2	1:D:167:SER:HB2	2.23	0.73
1:F:32:PRO:HA	1:F:150:MET:HE1	1.69	0.73
1:E:333:GLN:HE22	1:E:374:THR:CG2	2.02	0.73
1:E:333:GLN:HE22	1:E:374:THR:HG23	1.52	0.72
1:D:22:ARG:NH1	1:D:50:GLU:OE1	2.22	0.72
1:B:308:ALA:HB2	1:B:350:ILE:CD1	2.18	0.72
1:G:90:ARG:O	1:G:90:ARG:HG3	1.89	0.72
1:E:257:HIS:HE1	1:E:289:TYR:OH	1.72	0.72
1:F:359:GLN:HG2	1:C:18:ARG:HH22	1.54	0.72
1:F:257:HIS:HE1	1:F:289:TYR:OH	1.73	0.71
1:A:333:GLN:NE2	1:A:374:THR:CG2	2.48	0.71
1:G:103:TRP:CE3	1:G:107:ARG:NH1	2.59	0.71
1:A:296:ILE:HG23	1:A:302:MET:HE3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:HIS:HE1	1:A:289:TYR:OH	1.74	0.71
1:D:402:ALA:O	1:D:406:ILE:HG12	1.89	0.71
1:E:338:ARG:NH2	1:G:334:LEU:HD21	2.06	0.71
1:G:257:HIS:HE1	1:G:289:TYR:OH	1.74	0.71
1:E:294[A]:PHE:CE1	1:G:294:PHE:HE2	2.09	0.71
1:F:147:VAL:O	1:F:170:THR:HG22	1.91	0.71
1:F:322:ILE:HG13	1:F:322:ILE:O	1.90	0.70
1:E:209:GLN:HG2	1:E:336:PHE:CD1	2.25	0.70
1:H:403:LEU:HD22	1:H:403:LEU:N	2.04	0.70
1:H:257:HIS:HE1	1:H:289:TYR:OH	1.75	0.70
1:A:417:GLN:NE2	1:E:145:PRO:HG3	2.07	0.70
1:C:257:HIS:HE1	1:C:289:TYR:OH	1.74	0.70
1:C:333:GLN:NE2	1:C:374:THR:CG2	2.50	0.69
1:B:55:LEU:CD2	1:B:57:MET:HG3	2.21	0.69
1:C:63:ALA:HA	1:C:90:ARG:NH2	2.08	0.69
1:B:308:ALA:CB	1:B:350:ILE:CD1	2.70	0.69
1:A:312:ASP:HB3	1:A:366:LEU:HD13	1.73	0.69
1:B:257:HIS:HE1	1:B:289:TYR:OH	1.75	0.69
1:H:232:HIS:HB3	1:H:302:MET:HE1	1.74	0.69
1:H:204:ASP:OD1	1:H:226:ARG:HG3	1.92	0.69
1:B:362:ILE:CD1	1:B:403:LEU:HB3	2.24	0.68
1:D:257:HIS:HE1	1:D:289:TYR:OH	1.76	0.68
1:G:22:ARG:NH1	1:G:50:GLU:OE1	2.27	0.68
1:A:232:HIS:HB3	1:A:302:MET:HE1	1.74	0.68
1:C:314:THR:CG2	1:C:376:ARG:HD2	2.24	0.68
1:C:215:ILE:HD11	1:C:351:ALA:HB3	1.74	0.68
1:C:205:GLY:HA2	1:C:228:ASP:O	1.94	0.68
1:G:64:SER:HB3	1:G:66:GLU:OE2	1.94	0.67
1:C:197:HIS:CD2	1:C:387:GLY:HA2	2.29	0.67
1:H:21:MET:HB2	1:H:113:ASP:HB2	1.77	0.67
1:F:187:PHE:HB3	1:F:214:ALA:HB1	1.76	0.67
1:B:21:MET:HB2	1:B:113:ASP:HB2	1.76	0.67
1:D:52:VAL:O	1:D:74:ARG:O	2.13	0.67
1:D:232:HIS:HB3	1:D:302:MET:HE1	1.77	0.67
1:E:314:THR:HG22	1:E:396:LEU:CD2	2.24	0.67
1:C:312:ASP:HB3	1:C:366:LEU:HD13	1.76	0.67
1:E:314:THR:CG2	1:E:396:LEU:HD22	2.24	0.67
1:D:90:ARG:HG3	1:D:90:ARG:O	1.93	0.67
1:H:205:GLY:HA2	1:H:228:ASP:O	1.95	0.66
1:D:417:GLN:HA	1:D:417:GLN:OE1	1.94	0.66
1:E:158:THR:HB	1:E:284:LEU:HD22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:SER:H	1:G:90:ARG:NH1	1.88	0.66
1:G:205:GLY:HA2	1:G:228:ASP:O	1.96	0.66
1:C:338:ARG:CZ	1:D:338:ARG:HD2	2.26	0.66
1:A:118:GLN:NE2	1:A:152:ASN:HD22	1.93	0.66
1:F:9:SER:OG	1:F:10:PRO:HD2	1.95	0.66
1:E:333:GLN:NE2	1:E:374:THR:HG22	2.10	0.66
1:C:185:GLU:HG2	1:C:214:ALA:HB2	1.76	0.66
1:F:208:LEU:CD2	1:F:303:VAL:HG22	2.25	0.66
1:B:314:THR:HG21	1:B:376:ARG:HH21	1.61	0.66
1:E:118:GLN:NE2	1:E:152:ASN:HD22	1.93	0.66
1:D:235:MET:CE	1:D:267:LEU:HB3	2.25	0.66
1:C:197:HIS:NE2	1:C:387:GLY:HA2	2.11	0.65
1:H:394:ARG:HH11	1:H:394:ARG:HG3	1.61	0.65
1:A:147:VAL:O	1:A:170:THR:HG22	1.94	0.65
1:B:194:ILE:HD11	1:B:351:ALA:HB1	1.79	0.65
1:F:333:GLN:NE2	1:F:374:THR:OG1	2.28	0.65
1:B:377:ALA:O	2:B:501:HOH:O	2.14	0.65
1:E:205:GLY:HA2	1:E:228:ASP:O	1.95	0.65
1:D:314:THR:CG2	1:D:376:ARG:HH11	2.09	0.65
1:F:118:GLN:NE2	1:F:152:ASN:HD22	1.94	0.65
1:H:194:ILE:HD11	1:H:351:ALA:HB1	1.79	0.65
1:C:34:PRO:HD2	1:C:150:MET:HE1	1.79	0.64
1:E:29:ALA:HA	1:E:180:PRO:HG2	1.77	0.64
1:C:208:LEU:HD12	1:C:303:VAL:CG2	2.26	0.64
1:B:118:GLN:NE2	1:B:152:ASN:HD22	1.96	0.64
1:C:294:PHE:HB3	1:D:342:ARG:HH22	1.61	0.64
1:E:146:ILE:O	1:E:170:THR:HG23	1.97	0.64
1:F:417:GLN:OE1	1:C:145:PRO:CG	2.46	0.64
1:F:312:ASP:HB3	1:F:366:LEU:HD13	1.80	0.64
1:B:55:LEU:HD21	1:B:57:MET:HG3	1.80	0.64
1:B:205:GLY:HA2	1:B:228:ASP:O	1.97	0.64
1:C:316:GLN:HG2	1:C:376:ARG:HB3	1.79	0.64
1:B:394:ARG:HG3	1:B:394:ARG:HH11	1.63	0.64
1:C:132:VAL:HG22	1:C:266:VAL:HB	1.80	0.64
1:A:384:THR:HG23	1:A:406:ILE:CD1	2.28	0.63
1:B:53:HIS:CE1	1:B:73:ARG:HH11	2.16	0.63
1:E:118:GLN:HE21	1:E:152:ASN:HD22	1.46	0.63
1:F:372:VAL:CG2	1:H:372:VAL:HG21	2.29	0.63
1:E:56:GLN:HE21	1:E:73:ARG:HH21	1.46	0.63
1:E:209:GLN:HG3	1:E:304:ALA:HA	1.79	0.63
1:G:118:GLN:NE2	1:G:152:ASN:HD22	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ARG:NH1	1:B:50:GLU:OE1	2.31	0.63
1:C:90:ARG:HG3	1:C:90:ARG:HH11	1.63	0.63
1:F:338:ARG:CZ	1:H:338:ARG:HD2	2.27	0.63
1:C:118:GLN:NE2	1:C:152:ASN:HD22	1.96	0.63
1:D:226:ARG:HH11	1:D:226:ARG:HG3	1.62	0.63
1:F:322:ILE:O	1:F:322:ILE:CG1	2.47	0.63
1:H:118:GLN:NE2	1:H:152:ASN:HD22	1.97	0.63
1:F:80:PRO:HA	1:F:83:ARG:NH1	2.14	0.63
1:F:314:THR:CG2	1:F:376:ARG:HH11	2.11	0.63
1:C:209:GLN:HG3	1:C:304:ALA:HA	1.80	0.63
1:E:132:VAL:HG22	1:E:266:VAL:HB	1.80	0.63
1:B:72:ARG:HD3	1:B:92:ASP:OD2	1.99	0.62
1:D:209:GLN:HG3	1:D:336:PHE:CD1	2.34	0.62
1:E:209:GLN:HE22	1:E:306:ASN:ND2	1.93	0.62
1:B:317:VAL:HG11	1:B:350:ILE:HD13	1.82	0.62
1:D:235:MET:HE1	1:D:267:LEU:HB3	1.79	0.62
1:E:338:ARG:HH21	1:G:334:LEU:HD21	1.64	0.62
1:F:422:ARG:CB	1:F:422:ARG:HH11	2.12	0.62
1:E:34:PRO:HD2	1:E:150:MET:HE1	1.81	0.62
1:F:65:LEU:O	1:F:68:GLU:HG3	1.99	0.62
1:D:234:GLU:OE2	1:D:332:GLY:HA3	1.99	0.62
1:G:349:ILE:HD13	1:G:381:TYR:HB2	1.82	0.62
1:A:209:GLN:HE22	1:A:306:ASN:ND2	1.95	0.62
1:A:314:THR:HG22	1:A:396:LEU:HD22	1.81	0.62
1:F:205:GLY:HA2	1:F:228:ASP:O	1.99	0.62
1:B:384:THR:OG1	1:B:406:ILE:HG23	1.98	0.62
1:D:190:VAL:O	1:D:194:ILE:HG22	2.00	0.61
1:D:205:GLY:HA2	1:D:228:ASP:O	1.99	0.61
1:E:94:VAL:HG12	1:E:96:VAL:CG2	2.30	0.61
1:B:154:ARG:HD2	1:B:176:ASP:OD1	1.99	0.61
1:G:246:LYS:HB2	1:G:248:LEU:HD22	1.80	0.61
1:B:308:ALA:HB3	1:B:350:ILE:HD11	1.83	0.61
1:F:83:ARG:NH2	1:F:327:TYR:CE2	2.66	0.61
1:H:382:VAL:HG23	1:H:391:LEU:HD22	1.82	0.61
1:F:55:LEU:CD2	1:F:57:MET:HG3	2.31	0.61
1:C:29:ALA:HA	1:C:180:PRO:HG2	1.83	0.61
1:D:118:GLN:NE2	1:D:152:ASN:HD22	1.98	0.61
1:F:232:HIS:CD2	1:F:262:VAL:HG11	2.36	0.61
1:C:224:GLU:OE2	1:C:246:LYS:NZ	2.34	0.61
1:E:363:VAL:HG12	1:E:365:PHE:O	2.01	0.61
1:A:338:ARG:CZ	1:B:338:ARG:HD2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:154:ARG:NH1	1:H:176:ASP:OD1	2.34	0.60
1:A:34:PRO:HD2	1:A:150:MET:HE1	1.82	0.60
1:G:209:GLN:HG3	1:G:336:PHE:CD1	2.36	0.60
1:H:209:GLN:HG3	1:H:336:PHE:CD1	2.36	0.60
1:C:146:ILE:O	1:C:170:THR:HG23	2.01	0.60
1:F:372:VAL:HG21	1:H:372:VAL:CG2	2.32	0.60
1:H:384:THR:OG1	1:H:406:ILE:HG23	2.01	0.60
1:A:209:GLN:HG3	1:A:304:ALA:HA	1.83	0.60
1:G:417:GLN:OE1	1:G:427:ARG:NH2	2.31	0.60
1:A:229:LEU:HB2	1:A:248:LEU:O	2.00	0.60
1:B:209:GLN:HG3	1:B:336:PHE:CD1	2.36	0.60
1:E:94:VAL:HG12	1:E:96:VAL:HG23	1.84	0.60
1:G:385:GLU:HG2	1:G:386:TRP:CE3	2.35	0.60
1:F:29:ALA:HA	1:F:180:PRO:HG2	1.84	0.60
1:H:31:THR:HG21	1:H:57:MET:O	2.00	0.60
1:A:205:GLY:HA2	1:A:228:ASP:O	2.02	0.60
1:E:333:GLN:NE2	1:E:373:VAL:HG22	2.17	0.60
1:C:37:LYS:NZ	1:C:59:GLU:OE2	2.34	0.60
1:G:184:ARG:H	1:G:184:ARG:HD3	1.67	0.59
1:F:187:PHE:HE1	1:F:192:ARG:HG3	1.67	0.59
1:F:203:GLU:OE1	1:F:301:LYS:HE3	2.02	0.59
1:C:62:PHE:O	1:C:63:ALA:C	2.45	0.59
1:H:194:ILE:HD11	1:H:215:ILE:HD13	1.83	0.59
1:G:63:ALA:O	1:G:64:SER:CB	2.49	0.59
1:C:409:PRO:HA	1:C:412:ARG:HG3	1.84	0.59
1:E:294[A]:PHE:CE1	1:G:294:PHE:CE2	2.90	0.59
1:G:190:VAL:O	1:G:194:ILE:HG22	2.03	0.59
1:G:384:THR:OG1	1:G:406:ILE:HG23	2.03	0.59
1:F:208:LEU:CD2	1:F:303:VAL:CG2	2.79	0.59
1:A:208:LEU:HD12	1:A:303:VAL:CG2	2.33	0.59
1:B:232:HIS:HB3	1:B:302:MET:HE1	1.83	0.59
1:C:207:THR:O	1:C:302:MET:HE3	2.03	0.59
1:D:29:ALA:HA	1:D:180:PRO:HG2	1.83	0.59
1:F:229:LEU:HB2	1:F:248:LEU:O	2.03	0.58
1:C:76:LEU:N	1:C:76:LEU:HD12	2.18	0.58
1:E:83:ARG:NH2	1:E:327:TYR:CE2	2.71	0.58
1:H:314:THR:CG2	1:H:376:ARG:HH11	2.16	0.58
1:H:78:VAL:O	1:H:328:SER:HA	2.03	0.58
1:C:338:ARG:HH22	1:D:334:LEU:HD21	1.65	0.58
1:D:409:PRO:HA	1:D:412:ARG:HG3	1.84	0.58
1:H:54:LEU:O	1:H:55:LEU:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:394:ARG:HG3	1:G:394:ARG:HH11	1.68	0.58
1:B:8:THR:OG1	1:B:12:ASP:HB2	2.03	0.58
1:G:105:PHE:HB3	1:G:143:THR:HG21	1.84	0.58
1:F:207:THR:O	1:F:302:MET:HE3	2.03	0.58
1:B:29:ALA:HA	1:B:180:PRO:HG2	1.85	0.58
1:C:210:MET:HE1	1:C:220:LEU:HD13	1.84	0.58
1:F:384:THR:HG23	1:F:406:ILE:CD1	2.32	0.58
1:A:29:ALA:HA	1:A:180:PRO:HG2	1.85	0.58
1:B:194:ILE:HD11	1:B:215:ILE:HD13	1.85	0.58
1:C:83:ARG:NH2	1:C:327:TYR:CE2	2.72	0.58
1:F:209:GLN:HE22	1:F:306:ASN:ND2	1.98	0.57
1:H:210:MET:HE1	1:H:220:LEU:HD13	1.84	0.57
1:B:78:VAL:O	1:B:328:SER:HA	2.04	0.57
1:E:321:SER:HB2	1:E:323:GLY:O	2.03	0.57
1:G:29:ALA:HA	1:G:180:PRO:HG2	1.85	0.57
1:G:78:VAL:O	1:G:328:SER:HA	2.04	0.57
1:H:422:ARG:HH11	1:H:422:ARG:HG2	1.69	0.57
1:A:118:GLN:HE21	1:A:152:ASN:HD22	1.52	0.57
1:C:314:THR:HG22	1:C:376:ARG:HD2	1.85	0.57
1:C:319:ALA:CB	1:C:373:VAL:HG11	2.32	0.57
1:E:55:LEU:CD2	1:E:57:MET:HG3	2.34	0.57
1:E:208:LEU:HD12	1:E:303:VAL:CG2	2.34	0.57
1:E:294[B]:PHE:CE1	1:E:342:ARG:NH1	2.72	0.57
1:F:422:ARG:HH11	1:F:422:ARG:HB2	1.70	0.57
1:A:55:LEU:CD2	1:A:57:MET:HG3	2.35	0.57
1:D:83:ARG:NH2	1:D:327:TYR:CE2	2.73	0.57
1:D:207:THR:HG23	1:D:300:ARG:O	2.05	0.57
1:F:372:VAL:HG21	1:H:372:VAL:HG21	1.87	0.57
1:C:186:GLY:O	1:C:187:PHE:HB2	2.05	0.57
1:G:235:MET:CE	1:G:267:LEU:HB3	2.34	0.57
1:D:90:ARG:O	1:D:90:ARG:CG	2.52	0.57
1:E:232:HIS:CD2	1:E:262:VAL:HG11	2.40	0.57
1:E:407:ALA:O	1:E:412:ARG:NH1	2.38	0.57
1:B:229:LEU:HB2	1:B:248:LEU:O	2.04	0.57
1:G:129:SER:OG	1:G:162:THR:CG2	2.52	0.57
1:D:78:VAL:O	1:D:328:SER:HA	2.05	0.56
1:G:211:GLY:O	1:G:212:ILE:O	2.22	0.56
1:H:83:ARG:NH2	1:H:327:TYR:CE2	2.73	0.56
1:E:33:THR:CG2	1:E:177:TRP:CH2	2.88	0.56
1:F:76:LEU:N	1:F:76:LEU:HD12	2.19	0.56
1:H:207:THR:CG2	1:H:300:ARG:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:THR:O	1:D:162:THR:HG22	2.05	0.56
1:B:232:HIS:CD2	1:B:262:VAL:HG11	2.41	0.56
1:C:209:GLN:NE2	1:C:306:ASN:OD1	2.39	0.56
1:E:229:LEU:HB2	1:E:248:LEU:O	2.05	0.56
1:H:52:VAL:HG12	1:H:76:LEU:HD21	1.88	0.56
1:A:422:ARG:HD3	1:A:424:LEU:HD22	1.87	0.56
1:F:187:PHE:CB	1:F:214:ALA:HB1	2.36	0.56
1:F:314:THR:HG21	1:F:376:ARG:NH1	2.19	0.56
1:D:232:HIS:CD2	1:D:262:VAL:HG11	2.41	0.55
1:E:366:LEU:H	1:E:366:LEU:HD12	1.70	0.55
1:C:118:GLN:HE21	1:C:152:ASN:HD22	1.53	0.55
1:G:404:ILE:HG21	1:G:416:LEU:CD1	2.37	0.55
1:A:146:ILE:O	1:A:170:THR:HB	2.06	0.55
1:C:284:LEU:N	1:C:284:LEU:HD12	2.22	0.55
1:F:132:VAL:HG22	1:F:266:VAL:HB	1.88	0.55
1:A:83:ARG:NH2	1:A:327:TYR:CE2	2.74	0.55
1:A:158:THR:HB	1:A:284:LEU:HD22	1.88	0.55
1:A:187:PHE:HE1	1:A:192:ARG:CZ	2.20	0.55
1:D:207:THR:CG2	1:D:300:ARG:O	2.55	0.55
1:F:359:GLN:HG2	1:C:18:ARG:NH2	2.21	0.55
1:E:78:VAL:O	1:E:328:SER:HA	2.06	0.55
1:E:409:PRO:HA	1:E:412:ARG:HG3	1.88	0.55
1:G:409:PRO:HA	1:G:412:ARG:HG3	1.87	0.55
1:H:118:GLN:HE21	1:H:152:ASN:HD22	1.53	0.55
1:H:424:LEU:O	1:H:425:LEU:C	2.49	0.55
1:A:407:ALA:O	1:A:412:ARG:NH1	2.40	0.55
1:B:308:ALA:CB	1:B:350:ILE:HD11	2.37	0.55
1:D:129:SER:OG	1:D:162:THR:CG2	2.54	0.55
1:D:207:THR:HA	1:D:230:GLY:O	2.07	0.55
1:F:409:PRO:HA	1:F:412:ARG:HG3	1.89	0.54
1:D:236:ILE:HB	1:D:266:VAL:HG22	1.88	0.54
1:G:210:MET:H	1:G:233:THR:HG23	1.72	0.54
1:H:284:LEU:HD12	1:H:284:LEU:N	2.22	0.54
1:D:350:ILE:HD12	2:D:506:HOH:O	2.07	0.54
1:G:404:ILE:HG21	1:G:416:LEU:HD12	1.89	0.54
1:F:118:GLN:HE21	1:F:152:ASN:HD22	1.54	0.54
1:H:232:HIS:CD2	1:H:262:VAL:HG11	2.42	0.54
1:C:198:VAL:O	1:C:201:LEU:HB2	2.08	0.54
1:F:209:GLN:HG3	1:F:304:ALA:HA	1.89	0.54
1:H:207:THR:HG23	1:H:300:ARG:O	2.08	0.54
1:C:229:LEU:HB2	1:C:248:LEU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:THR:HG21	1:D:376:ARG:NH1	2.21	0.54
1:E:294[B]:PHE:HE2	1:G:342:ARG:HD3	1.73	0.54
1:G:229:LEU:HB2	1:G:248:LEU:O	2.07	0.54
1:F:322:ILE:O	1:F:323:GLY:O	2.26	0.54
1:E:33:THR:HG23	1:E:177:TRP:CH2	2.43	0.54
1:F:92:ASP:OD2	1:H:397:ARG:HD2	2.07	0.54
1:G:322:ILE:HG13	1:G:327:TYR:CD1	2.42	0.54
1:H:394:ARG:HH11	1:H:394:ARG:CG	2.21	0.54
1:A:348:PRO:HG2	1:A:380:HIS:CG	2.43	0.54
1:H:22:ARG:NH1	1:H:50:GLU:OE1	2.40	0.54
1:F:348:PRO:HG2	1:F:380:HIS:CG	2.43	0.54
1:H:409:PRO:HA	1:H:412:ARG:HG3	1.90	0.54
1:A:409:PRO:HA	1:A:412:ARG:HG3	1.89	0.54
1:B:201:LEU:O	1:B:347:ARG:NH1	2.39	0.54
1:D:226:ARG:O	1:D:248:LEU:HD12	2.07	0.54
1:D:380:HIS:CE1	1:D:392:PHE:CG	2.95	0.54
1:H:229:LEU:HB2	1:H:248:LEU:O	2.08	0.53
1:G:21:MET:HA	1:G:113:ASP:OD2	2.08	0.53
1:G:279:ASN:OD1	1:G:281:LEU:HB2	2.08	0.53
1:B:366:LEU:HG	2:B:503:HOH:O	2.08	0.53
1:B:380:HIS:CE1	1:B:392:PHE:CG	2.97	0.53
1:D:348:PRO:HG2	1:D:380:HIS:CG	2.43	0.53
1:E:260:LYS:CE	1:E:280:PRO:O	2.56	0.53
1:E:294[B]:PHE:HE1	1:E:342:ARG:NH1	2.07	0.53
1:G:203:GLU:OE1	1:G:301:LYS:HE3	2.09	0.53
1:F:21:MET:HA	1:F:113:ASP:OD2	2.09	0.53
1:C:323:GLY:CA	1:C:370:ALA:HA	2.24	0.53
1:D:201:LEU:O	1:D:347:ARG:NH1	2.42	0.53
1:G:232:HIS:CD2	1:G:262:VAL:HG11	2.43	0.53
1:G:234:GLU:OE2	1:G:291:ASN:ND2	2.34	0.53
1:B:423:GLY:C	1:B:424:LEU:HG	2.31	0.53
1:E:60:ASP:OD2	1:E:63:ALA:HB2	2.09	0.53
1:E:348:PRO:HG2	1:E:380:HIS:CG	2.44	0.53
1:H:76:LEU:HD12	1:H:94:VAL:HG13	1.91	0.53
1:B:56:GLN:HE21	1:B:73:ARG:HH12	1.57	0.53
1:C:134:VAL:O	1:C:135:ILE:C	2.52	0.53
1:D:229:LEU:HB2	1:D:248:LEU:O	2.08	0.53
1:G:380:HIS:CE1	1:G:392:PHE:CG	2.97	0.53
1:H:207:THR:HA	1:H:230:GLY:O	2.08	0.53
1:A:21:MET:HA	1:A:113:ASP:OD2	2.09	0.53
1:B:118:GLN:HE21	1:B:152:ASN:HD22	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:PRO:HA	1:B:412:ARG:HG3	1.89	0.53
1:E:316:GLN:HG2	1:E:376:ARG:HB3	1.91	0.53
1:E:372:VAL:H	1:G:316:GLN:HE22	1.57	0.53
1:D:279:ASN:OD1	1:D:281:LEU:HB2	2.09	0.53
1:H:364:PRO:O	1:H:422:ARG:NE	2.41	0.52
1:C:21:MET:HA	1:C:113:ASP:OD2	2.09	0.52
1:C:260:LYS:CE	1:C:280:PRO:O	2.56	0.52
1:G:11:GLU:CD	1:G:11:GLU:H	2.17	0.52
1:G:55:LEU:CD2	1:G:57:MET:HG3	2.39	0.52
1:G:60:ASP:OD2	1:G:63:ALA:HB2	2.08	0.52
1:F:314:THR:CG2	1:F:316:GLN:HG3	2.39	0.52
1:H:380:HIS:CE1	1:H:392:PHE:CG	2.96	0.52
1:B:83:ARG:NH2	1:B:327:TYR:CZ	2.78	0.52
1:E:21:MET:HA	1:E:113:ASP:OD2	2.10	0.52
1:E:134:VAL:O	1:E:135:ILE:C	2.53	0.52
1:A:6:LYS:HD3	1:A:169:PHE:O	2.10	0.52
1:A:60:ASP:OD2	1:A:63:ALA:HB2	2.10	0.52
1:C:78:VAL:O	1:C:328:SER:HA	2.09	0.52
1:D:21:MET:HA	1:D:113:ASP:OD2	2.10	0.52
1:E:260:LYS:HE3	1:E:280:PRO:O	2.09	0.52
1:G:207:THR:HA	1:G:230:GLY:O	2.10	0.52
1:H:134:VAL:O	1:H:135:ILE:C	2.52	0.52
1:A:359:GLN:NE2	1:E:18:ARG:NH2	2.57	0.52
1:C:348:PRO:HG2	1:C:380:HIS:CG	2.45	0.52
1:G:348:PRO:HG2	1:G:380:HIS:CG	2.45	0.52
1:D:209:GLN:HG3	1:D:336:PHE:CE1	2.44	0.52
1:F:146:ILE:O	1:F:170:THR:HB	2.09	0.52
1:D:384:THR:CG2	1:D:406:ILE:HG22	2.40	0.52
1:E:59:GLU:O	1:E:60:ASP:CB	2.55	0.52
1:E:207:THR:O	1:E:302:MET:HE3	2.10	0.52
1:E:382:VAL:HG23	1:E:391:LEU:HD22	1.90	0.52
1:F:316:GLN:HE22	1:H:372:VAL:H	1.56	0.52
1:H:241:LEU:HD21	1:H:271:ARG:NH2	2.24	0.52
1:A:3:TYR:CE1	1:A:122:PRO:HG3	2.45	0.52
1:A:316:GLN:HG2	1:A:376:ARG:HB3	1.91	0.52
1:D:210:MET:H	1:D:233:THR:HG23	1.75	0.52
1:D:276:VAL:HG23	1:D:282:PHE:CD2	2.45	0.52
1:B:314:THR:CG2	1:B:316:GLN:HG3	2.40	0.52
1:B:317:VAL:CG1	1:B:350:ILE:HD13	2.39	0.52
1:F:134:VAL:O	1:F:135:ILE:C	2.53	0.51
1:B:284:LEU:N	1:B:284:LEU:HD12	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:SER:OG	1:G:162:THR:HG21	2.09	0.51
1:F:183:LYS:H	1:F:183:LYS:HD2	1.74	0.51
1:F:316:GLN:HG2	1:F:376:ARG:HB3	1.92	0.51
1:B:134:VAL:O	1:B:135:ILE:C	2.53	0.51
1:B:207:THR:HA	1:B:230:GLY:O	2.11	0.51
1:D:118:GLN:HE21	1:D:152:ASN:HD22	1.58	0.51
1:G:162:THR:HG22	1:G:162:THR:O	2.09	0.51
1:F:284:LEU:HD12	1:F:284:LEU:N	2.25	0.51
1:A:198:VAL:O	1:A:201:LEU:HB2	2.10	0.51
1:E:207:THR:HA	1:E:230:GLY:O	2.10	0.51
1:G:118:GLN:HE21	1:G:152:ASN:HD22	1.56	0.51
1:C:241:LEU:HD21	1:C:271:ARG:NH2	2.25	0.51
1:E:198:VAL:O	1:E:201:LEU:HB2	2.11	0.51
1:H:7:LEU:HD12	1:H:172:ILE:HG22	1.91	0.51
1:C:380:HIS:CE1	1:C:392:PHE:CG	2.97	0.51
1:H:384:THR:HG23	1:H:406:ILE:CG2	2.41	0.51
1:F:208:LEU:HD22	1:F:303:VAL:CG2	2.41	0.51
1:C:372:VAL:H	1:D:316:GLN:HE22	1.59	0.51
1:B:83:ARG:NH2	1:B:327:TYR:CE2	2.79	0.51
1:H:194:ILE:CD1	1:H:215:ILE:HD13	2.41	0.51
1:A:134:VAL:O	1:A:135:ILE:C	2.54	0.51
1:A:419:ALA:O	1:A:422:ARG:O	2.28	0.51
1:D:412:ARG:O	1:D:416:LEU:HB2	2.11	0.51
1:B:279:ASN:OD1	1:B:281:LEU:HB2	2.11	0.51
1:H:189:GLU:OE1	1:H:192:ARG:HD2	2.12	0.50
1:F:103:TRP:HB3	1:F:107:ARG:CD	2.39	0.50
1:H:314:THR:CG2	1:H:316:GLN:HG3	2.40	0.50
1:C:207:THR:HA	1:C:230:GLY:O	2.12	0.50
1:G:419:ALA:CB	1:G:425:LEU:HD21	2.41	0.50
1:F:198:VAL:O	1:F:201:LEU:HB2	2.11	0.50
1:H:276:VAL:HG23	1:H:282:PHE:CD2	2.46	0.50
1:G:134:VAL:O	1:G:135:ILE:C	2.54	0.50
1:F:338:ARG:NH2	1:H:334:LEU:HD21	2.26	0.50
1:F:372:VAL:H	1:H:316:GLN:HE22	1.58	0.50
1:A:372:VAL:H	1:B:316:GLN:HE22	1.58	0.50
1:D:382:VAL:HG23	1:D:391:LEU:HD22	1.94	0.50
1:G:103:TRP:CZ3	1:G:107:ARG:NH1	2.79	0.50
1:G:296:ILE:HG12	1:G:339:GLY:CA	2.38	0.50
1:F:338:ARG:HD3	1:H:338:ARG:CZ	2.42	0.50
1:H:207:THR:HG21	1:H:299:ASN:HB3	1.93	0.50
1:H:236:ILE:HB	1:H:266:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:279:ASN:OD1	1:H:281:LEU:HB2	2.11	0.50
1:E:417:GLN:OE1	1:E:417:GLN:HA	2.11	0.50
1:G:276:VAL:HG23	1:G:282:PHE:CD2	2.47	0.50
1:B:348:PRO:HG2	1:B:380:HIS:CG	2.46	0.50
1:E:4:ARG:O	1:E:6:LYS:N	2.39	0.50
1:G:209:GLN:HG3	1:G:336:PHE:CE1	2.47	0.50
1:H:348:PRO:HG2	1:H:380:HIS:CG	2.47	0.50
1:A:322:ILE:O	1:A:323:GLY:O	2.30	0.50
1:A:210:MET:HE3	1:A:305:ILE:HD12	1.93	0.49
1:A:276:VAL:HG12	1:A:282:PHE:CE2	2.47	0.49
1:D:363:VAL:HG22	1:D:364:PRO:HD2	1.94	0.49
1:G:210:MET:HE1	1:G:220:LEU:HD13	1.94	0.49
1:F:32:PRO:CB	1:F:150:MET:CE	2.90	0.49
1:A:88[B]:GLN:HG2	1:A:90:ARG:HG2	1.94	0.49
1:B:198:VAL:O	1:B:201:LEU:HB2	2.12	0.49
1:G:235:MET:HE1	1:G:267:LEU:HB3	1.94	0.49
1:G:412:ARG:O	1:G:416:LEU:HD13	2.12	0.49
1:F:382:VAL:HG23	1:F:391:LEU:CD2	2.42	0.49
1:H:198:VAL:O	1:H:201:LEU:HB2	2.13	0.49
1:A:382:VAL:HG23	1:A:391:LEU:CD2	2.42	0.49
1:B:63:ALA:O	1:B:90:ARG:NH2	2.45	0.49
1:G:158:THR:HB	1:G:284:LEU:HD12	1.93	0.49
1:C:215:ILE:CD1	1:C:351:ALA:HB3	2.39	0.49
1:E:319:ALA:CB	1:E:373:VAL:HG11	2.35	0.49
1:F:207:THR:HA	1:F:230:GLY:O	2.12	0.49
1:H:416:LEU:O	1:H:420:TRP:HD1	1.96	0.49
1:A:353:PRO:O	1:A:361:ARG:HD2	2.13	0.49
1:B:184:ARG:NH2	1:B:186:GLY:HA2	2.27	0.49
1:C:276:VAL:HG12	1:C:282:PHE:CE2	2.48	0.49
1:B:37:LYS:NZ	1:B:59:GLU:OE2	2.35	0.49
1:F:294:PHE:CE1	1:F:342:ARG:NH1	2.81	0.49
1:H:349:ILE:HD13	1:H:381:TYR:HB2	1.95	0.49
1:A:333:GLN:HE21	1:A:374:THR:HG21	1.66	0.49
1:D:105:PHE:HB3	1:D:143:THR:HG21	1.94	0.49
1:D:314:THR:CG2	1:D:316:GLN:HG3	2.43	0.49
1:G:315:GLY:O	1:G:379:VAL:HG21	2.12	0.49
1:H:227:ARG:HA	1:H:227:ARG:HD3	1.52	0.49
1:A:203:GLU:HG3	1:A:301:LYS:NZ	2.27	0.49
1:D:65:LEU:HA	1:D:90:ARG:NH2	2.28	0.49
1:F:338:ARG:HD3	1:H:338:ARG:NH1	2.28	0.49
1:A:224:GLU:HA	1:A:224:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294[B]:PHE:HD2	1:G:342:ARG:NH1	2.09	0.49
1:G:322:ILE:O	1:G:323:GLY:O	2.31	0.49
1:B:382:VAL:HG23	1:B:391:LEU:CD2	2.42	0.48
1:D:134:VAL:O	1:D:135:ILE:C	2.55	0.48
1:E:276:VAL:HG12	1:E:282:PHE:CE2	2.48	0.48
1:F:294:PHE:HZ	1:H:293:PRO:HB2	1.78	0.48
1:H:209:GLN:HG3	1:H:336:PHE:CE1	2.48	0.48
1:H:216:PRO:HG3	1:H:305:ILE:HD11	1.95	0.48
1:H:403:LEU:CD2	1:H:403:LEU:N	2.74	0.48
1:A:88[B]:GLN:CD	1:A:90:ARG:HG3	2.38	0.48
1:B:194:ILE:CD1	1:B:215:ILE:HD13	2.43	0.48
1:G:8:THR:HG21	1:G:171:ALA:HB1	1.94	0.48
1:G:234:GLU:OE1	1:G:332:GLY:HA3	2.13	0.48
1:G:363:VAL:HG22	1:G:364:PRO:HD2	1.95	0.48
1:F:155:MET:SD	1:F:156:PRO:HD2	2.53	0.48
1:A:315:GLY:O	1:A:379:VAL:HG21	2.13	0.48
1:A:383:VAL:HG22	1:A:388:VAL:HG22	1.95	0.48
1:G:384:THR:HG23	1:G:406:ILE:CG2	2.43	0.48
1:F:60:ASP:OD2	1:F:63:ALA:HB2	2.13	0.48
1:F:212:ILE:HG13	1:F:213:GLY:H	1.78	0.48
1:H:194:ILE:CD1	1:H:351:ALA:HB1	2.44	0.48
1:H:201:LEU:O	1:H:347:ARG:NH1	2.44	0.48
1:G:198:VAL:O	1:G:201:LEU:HB2	2.12	0.48
1:B:308:ALA:HB2	1:B:350:ILE:HD12	1.93	0.48
1:F:319:ALA:CB	1:F:373:VAL:HG11	2.33	0.48
1:E:257:HIS:CD2	1:E:283:GLU:OE2	2.66	0.48
1:G:254:LYS:O	1:G:255:SER:HB3	2.12	0.48
1:F:257:HIS:CD2	1:F:283:GLU:OE2	2.67	0.48
1:A:207:THR:HA	1:A:230:GLY:O	2.13	0.48
1:D:129:SER:OG	1:D:162:THR:HG21	2.13	0.48
1:H:296:ILE:HG12	1:H:339:GLY:CA	2.37	0.48
1:H:296:ILE:HD12	1:H:302:MET:HE3	1.96	0.48
1:B:18:ARG:O	1:B:21:MET:HG2	2.14	0.48
1:C:233:THR:HG21	1:C:235:MET:O	2.14	0.48
1:D:52:VAL:O	1:D:53:HIS:CG	2.66	0.48
1:G:9:SER:OG	1:G:12:ASP:OD1	2.31	0.48
1:G:155:MET:SD	1:G:156:PRO:HD2	2.53	0.48
1:H:155:MET:SD	1:H:156:PRO:HD2	2.54	0.48
1:A:132:VAL:HG22	1:A:266:VAL:HB	1.96	0.48
1:B:9:SER:OG	1:B:12:ASP:OD1	2.32	0.48
1:B:192:ARG:O	1:B:196:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:MET:SD	1:D:156:PRO:HD2	2.53	0.48
1:D:235:MET:HE3	1:D:267:LEU:HB3	1.95	0.48
1:E:314:THR:HG21	1:E:376:ARG:NH1	2.28	0.48
1:E:316:GLN:HE22	1:G:372:VAL:H	1.61	0.48
1:G:236:ILE:HB	1:G:266:VAL:HG22	1.95	0.47
1:G:383:VAL:HG22	1:G:388:VAL:HG22	1.96	0.47
1:F:276:VAL:HG12	1:F:282:PHE:CE2	2.50	0.47
1:C:155:MET:SD	1:C:156:PRO:HD2	2.55	0.47
1:C:322:ILE:O	1:C:323:GLY:O	2.32	0.47
1:G:235:MET:HE3	1:G:267:LEU:HB3	1.97	0.47
1:G:257:HIS:CD2	1:G:283:GLU:OE2	2.68	0.47
1:H:238:ASP:OD1	1:H:268:GLY:HA3	2.14	0.47
1:B:209:GLN:HG3	1:B:336:PHE:CE1	2.49	0.47
1:G:29:ALA:HB3	1:G:132:VAL:HG21	1.97	0.47
1:C:234:GLU:OE1	1:C:332:GLY:HA3	2.15	0.47
1:E:315:GLY:O	1:E:379:VAL:HG21	2.15	0.47
1:H:18:ARG:O	1:H:21:MET:HG2	2.14	0.47
1:A:64:SER:CB	1:A:66:GLU:OE2	2.63	0.47
1:B:181:GLU:HG2	1:B:269:SER:HA	1.96	0.47
1:G:53:HIS:HD2	1:G:54:LEU:O	1.97	0.47
1:G:212:ILE:HG13	1:G:213:GLY:H	1.78	0.47
1:G:419:ALA:HB3	1:G:425:LEU:HD21	1.97	0.47
1:A:236:ILE:HB	1:A:266:VAL:HG22	1.96	0.47
1:B:383:VAL:HG22	1:B:388:VAL:HG22	1.97	0.47
1:C:294:PHE:HB3	1:D:342:ARG:NH2	2.28	0.47
1:D:187:PHE:HB2	1:D:191:GLU:CG	2.45	0.47
1:G:382:VAL:HG23	1:G:391:LEU:CD2	2.45	0.47
1:H:261:ILE:HD12	1:H:281:LEU:CD1	2.45	0.47
1:H:383:VAL:HG22	1:H:388:VAL:HG22	1.97	0.47
1:A:312:ASP:OD1	1:A:314:THR:OG1	2.26	0.47
1:B:209:GLN:HA	1:B:233:THR:CG2	2.30	0.47
1:C:315:GLY:O	1:C:379:VAL:HG21	2.15	0.47
1:D:416:LEU:HD12	1:D:425:LEU:HD11	1.97	0.47
1:F:32:PRO:C	1:F:150:MET:HE1	2.40	0.47
1:A:234:GLU:OE1	1:A:332:GLY:HA3	2.15	0.47
1:B:394:ARG:HH11	1:B:394:ARG:CG	2.27	0.47
1:C:168:ARG:HD2	1:C:168:ARG:HA	1.72	0.47
1:D:129:SER:OG	1:D:162:THR:HG22	2.15	0.47
1:D:158:THR:HB	1:D:284:LEU:HD22	1.97	0.47
1:G:53:HIS:HE1	1:G:73:ARG:HG2	1.80	0.47
1:G:184:ARG:HD3	1:G:184:ARG:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:ARG:HG3	1:F:72:ARG:HH11	1.78	0.46
1:B:316:GLN:HG2	1:B:376:ARG:HB3	1.97	0.46
1:E:146:ILE:O	1:E:170:THR:CG2	2.63	0.46
1:G:216:PRO:HG3	1:G:305:ILE:HD11	1.97	0.46
1:B:21:MET:HA	1:B:113:ASP:OD2	2.16	0.46
1:B:258:PRO:O	2:B:502:HOH:O	2.20	0.46
1:B:384:THR:HG23	1:B:406:ILE:CG2	2.45	0.46
1:C:253[A]:LYS:HZ2	1:C:253[A]:LYS:HG2	1.45	0.46
1:C:408:HIS:ND1	1:C:409:PRO:HD2	2.30	0.46
1:D:31:THR:CG2	1:D:57:MET:O	2.47	0.46
1:D:315:GLY:O	1:D:379:VAL:HG21	2.15	0.46
1:F:80:PRO:CA	1:F:83:ARG:HH11	2.26	0.46
1:H:21:MET:HE2	1:H:113:ASP:HB3	1.98	0.46
1:H:55:LEU:HD23	1:H:56:GLN:H	1.80	0.46
1:H:76:LEU:HD12	1:H:94:VAL:CG1	2.46	0.46
1:A:155:MET:SD	1:A:156:PRO:HD2	2.55	0.46
1:B:362:ILE:HD11	1:B:403:LEU:HB3	1.98	0.46
1:C:383:VAL:HG22	1:C:388:VAL:HG22	1.96	0.46
1:G:215:ILE:HD11	1:G:353:PRO:HD3	1.97	0.46
1:F:333:GLN:HE21	1:F:374:THR:HG1	1.60	0.46
1:A:408:HIS:ND1	1:A:409:PRO:HD2	2.30	0.46
1:E:408:HIS:ND1	1:E:409:PRO:HD2	2.31	0.46
1:C:33:THR:OG1	1:C:177:TRP:HZ2	1.94	0.46
1:C:97:MET:HE1	1:D:378:ASP:OD1	2.16	0.46
1:C:382:VAL:HG23	1:C:391:LEU:CD2	2.46	0.46
1:D:103:TRP:CE3	1:D:107:ARG:NH2	2.84	0.46
1:D:158:THR:OG1	1:D:162:THR:HG21	2.15	0.46
1:D:207:THR:HG21	1:D:299:ASN:HB3	1.97	0.46
1:D:384:THR:HG23	1:D:406:ILE:CG2	2.45	0.46
1:G:408:HIS:ND1	1:G:409:PRO:HD2	2.31	0.46
1:A:146:ILE:HG23	1:A:170:THR:HG21	1.98	0.46
1:D:394:ARG:HG3	1:D:394:ARG:HH11	1.79	0.46
1:G:353:PRO:O	1:G:361:ARG:HD2	2.16	0.46
1:H:408:HIS:ND1	1:H:409:PRO:HD2	2.31	0.46
1:B:53:HIS:HE1	1:B:73:ARG:HH11	1.61	0.46
1:C:54:LEU:CD1	1:C:76:LEU:HB2	2.46	0.46
1:D:408:HIS:ND1	1:D:409:PRO:HD2	2.31	0.46
1:E:217:ASP:OD1	1:E:217:ASP:N	2.46	0.46
1:H:322:ILE:O	1:H:323:GLY:O	2.33	0.46
1:D:382:VAL:HG23	1:D:391:LEU:CD2	2.46	0.46
1:B:194:ILE:CD1	1:B:351:ALA:HB1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:ARG:CZ	1:D:192:ARG:HB3	2.45	0.46
1:D:215:ILE:HD11	1:D:353:PRO:HD3	1.98	0.46
1:F:169:PHE:HB2	1:F:172:ILE:HD11	1.97	0.46
1:A:146:ILE:O	1:A:170:THR:CG2	2.63	0.46
1:D:198:VAL:O	1:D:201:LEU:HB2	2.15	0.46
1:E:234:GLU:OE1	1:E:332:GLY:HA3	2.16	0.46
1:F:408:HIS:ND1	1:F:409:PRO:HD2	2.31	0.45
1:B:382:VAL:HG23	1:B:391:LEU:HD22	1.97	0.45
1:B:408:HIS:ND1	1:B:409:PRO:HD2	2.30	0.45
1:E:163:PHE:HB2	2:E:503:HOH:O	2.16	0.45
1:G:129:SER:OG	1:G:162:THR:HG22	2.15	0.45
1:H:3:TYR:C	1:H:5:LYS:H	2.24	0.45
1:E:24:PHE:O	1:E:115:ALA:HA	2.17	0.45
1:E:155:MET:SD	1:E:156:PRO:HD2	2.56	0.45
1:B:184:ARG:HH21	1:B:186:GLY:HA2	1.81	0.45
1:C:297:ALA:HB2	1:C:342:ARG:HG3	1.98	0.45
1:C:384:THR:HG23	1:C:406:ILE:HD12	1.97	0.45
1:F:353:PRO:O	1:F:361:ARG:HD2	2.17	0.45
1:A:384:THR:CG2	1:A:406:ILE:CD1	2.94	0.45
1:G:332:GLY:O	1:G:333:GLN:C	2.59	0.45
1:F:146:ILE:O	1:F:170:THR:CG2	2.65	0.45
1:H:102:PRO:HG2	1:H:288:ASP:HB2	1.98	0.45
1:H:245:GLU:OE2	1:H:271:ARG:NH2	2.50	0.45
1:E:319:ALA:H	1:E:373:VAL:HG12	1.81	0.45
1:G:191:GLU:O	1:G:194:ILE:HG23	2.16	0.45
1:A:316:GLN:HE22	1:B:372:VAL:H	1.62	0.45
1:B:168:ARG:HD2	1:B:168:ARG:HA	1.67	0.45
1:G:350:ILE:HD13	1:G:379:VAL:HG13	1.99	0.45
1:H:21:MET:HA	1:H:113:ASP:OD2	2.17	0.45
1:B:276:VAL:HG23	1:B:282:PHE:CD2	2.52	0.45
1:B:315:GLY:O	1:B:379:VAL:HG21	2.16	0.45
1:G:8:THR:OG1	1:G:9:SER:N	2.50	0.45
1:G:158:THR:OG1	1:G:162:THR:HG21	2.16	0.45
1:B:279:ASN:OD1	1:B:279:ASN:C	2.60	0.45
1:C:257:HIS:CD2	1:C:283:GLU:OE2	2.70	0.45
1:D:24:PHE:CD1	1:D:24:PHE:C	2.95	0.45
1:D:183:LYS:HE2	1:D:183:LYS:HA	1.97	0.45
1:F:101:VAL:HB	1:F:102:PRO:HD3	1.99	0.44
1:A:187:PHE:HB2	1:A:191:GLU:HB2	1.99	0.44
1:B:332:GLY:O	1:B:333:GLN:C	2.61	0.44
1:E:294[B]:PHE:CD2	1:G:342:ARG:NH1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ILE:HD13	1:B:336:PHE:CD1	2.53	0.44
1:E:33:THR:OG1	1:E:34:PRO:HD3	2.18	0.44
1:E:58:GLY:O	1:E:59:GLU:C	2.61	0.44
1:E:342:ARG:HH22	1:G:294:PHE:HB3	1.82	0.44
1:F:383:VAL:HG22	1:F:388:VAL:HG22	2.00	0.44
1:B:302:MET:HE3	1:B:336:PHE:CE1	2.53	0.44
1:C:146:ILE:O	1:C:170:THR:CG2	2.64	0.44
1:C:342:ARG:NH2	1:D:292:ASP:OD1	2.50	0.44
1:C:382:VAL:HG23	1:C:391:LEU:HD22	1.98	0.44
1:E:9:SER:OG	1:E:12:ASP:OD1	2.35	0.44
1:G:241:LEU:HD21	1:G:271:ARG:NH1	2.33	0.44
1:A:401:LYS:HB3	1:A:401:LYS:HE3	1.55	0.44
1:A:417:GLN:NE2	1:E:145:PRO:CG	2.78	0.44
1:B:102:PRO:HG2	1:B:288:ASP:HB2	1.98	0.44
1:C:24:PHE:CD1	1:C:24:PHE:C	2.96	0.44
1:D:112:LEU:HD12	1:D:143:THR:CG2	2.48	0.44
1:D:316:GLN:HG2	1:D:376:ARG:HB3	1.99	0.44
1:G:158:THR:CB	1:G:284:LEU:HD12	2.47	0.44
1:C:34:PRO:HD2	1:C:150:MET:CE	2.47	0.44
1:D:279:ASN:OD1	1:D:279:ASN:C	2.59	0.44
1:D:305:ILE:HG13	1:D:305:ILE:O	2.18	0.44
1:H:24:PHE:CD1	1:H:24:PHE:C	2.95	0.44
1:A:209:GLN:NE2	1:A:306:ASN:HD21	1.99	0.44
1:C:323:GLY:CA	1:C:370:ALA:CA	2.91	0.44
1:H:296:ILE:HD13	1:H:336:PHE:CD1	2.53	0.44
1:D:24:PHE:O	1:D:115:ALA:HA	2.18	0.44
1:D:43:LYS:HB2	1:D:67:MET:HE3	2.00	0.44
1:G:18:ARG:NH1	1:G:18:ARG:HG2	2.32	0.44
1:H:279:ASN:OD1	1:H:279:ASN:C	2.60	0.44
1:E:209:GLN:NE2	1:E:306:ASN:HD21	1.97	0.44
1:G:296:ILE:HD13	1:G:336:PHE:HA	2.00	0.44
1:F:24:PHE:O	1:F:115:ALA:HA	2.18	0.44
1:F:25:VAL:HG11	1:F:36:LEU:HD21	1.99	0.44
1:H:296:ILE:HD13	1:H:336:PHE:HA	1.99	0.44
1:A:279:ASN:C	1:A:279:ASN:OD1	2.61	0.44
1:B:296:ILE:HG12	1:B:339:GLY:CA	2.37	0.44
1:C:35:LEU:HD23	1:C:116:ILE:HG23	1.99	0.44
1:D:96:VAL:HG13	1:D:96:VAL:O	2.17	0.44
1:D:349:ILE:HD13	1:D:381:TYR:CB	2.43	0.44
1:F:9:SER:OG	1:F:10:PRO:CD	2.65	0.43
1:F:186:GLY:O	1:F:187:PHE:CD2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:LYS:HE3	1:H:139:ALA:HB2	2.00	0.43
1:B:413:GLU:OE2	1:C:68:GLU:HB3	2.18	0.43
1:D:212:ILE:HG13	1:D:213:GLY:H	1.83	0.43
1:E:24:PHE:CD1	1:E:24:PHE:C	2.96	0.43
1:E:177:TRP:CD1	1:E:178:PRO:HD2	2.53	0.43
1:G:313:LEU:CD1	1:G:362:ILE:HD11	2.48	0.43
1:F:146:ILE:CG2	1:F:170:THR:HG21	2.48	0.43
1:C:334:LEU:HD13	1:C:338:ARG:NH1	2.34	0.43
1:D:43:LYS:HB2	1:D:67:MET:CE	2.49	0.43
1:G:235:MET:HE3	1:G:235:MET:HB2	1.84	0.43
1:F:208:LEU:HD23	1:F:303:VAL:CG2	2.37	0.43
1:F:294:PHE:CZ	1:H:294:PHE:HB2	2.53	0.43
1:F:384:THR:CG2	1:F:406:ILE:CD1	2.96	0.43
1:A:232:HIS:CE1	1:A:262:VAL:HG11	2.53	0.43
1:B:155:MET:SD	1:B:156:PRO:HD2	2.58	0.43
1:D:394:ARG:HH11	1:D:394:ARG:CG	2.31	0.43
1:G:56:GLN:HE21	1:G:73:ARG:NH1	2.16	0.43
1:F:342:ARG:O	1:F:342:ARG:HG2	2.18	0.43
1:A:24:PHE:O	1:A:115:ALA:HA	2.19	0.43
1:B:35:LEU:HD23	1:B:116:ILE:HG23	2.00	0.43
1:C:333:GLN:HE21	1:C:374:THR:HG22	1.70	0.43
1:E:334:LEU:HD13	1:E:338:ARG:NH1	2.33	0.43
1:G:101:VAL:HB	1:G:102:PRO:HD3	2.00	0.43
1:G:305:ILE:O	1:G:305:ILE:HG13	2.18	0.43
1:F:279:ASN:C	1:F:279:ASN:OD1	2.62	0.43
1:A:46:LEU:C	1:A:47:GLU:HG2	2.44	0.43
1:A:355:THR:O	2:A:501:HOH:O	2.21	0.43
1:A:359:GLN:HE21	1:A:359:GLN:HB3	1.43	0.43
1:B:284:LEU:N	1:B:284:LEU:CD1	2.82	0.43
1:D:355:THR:HA	1:D:359:GLN:O	2.19	0.43
1:G:384:THR:CG2	1:G:406:ILE:HG23	2.49	0.43
1:B:76:LEU:HD12	1:B:94:VAL:HG13	2.00	0.43
1:B:296:ILE:HD13	1:B:336:PHE:HA	2.00	0.43
1:C:203:GLU:OE2	1:C:301:LYS:HE3	2.18	0.43
1:G:296:ILE:HD12	1:G:302:MET:HE3	2.00	0.43
1:A:93:TYR:CE1	1:A:329:GLY:HA2	2.53	0.43
1:E:32:PRO:CB	1:E:150:MET:HE3	2.49	0.43
1:E:314:THR:HG21	1:E:376:ARG:HH11	1.83	0.43
1:G:56:GLN:HE21	1:G:73:ARG:HH12	1.65	0.43
1:G:64:SER:N	1:G:90:ARG:NH1	2.59	0.43
1:F:194:ILE:HG12	1:F:384:THR:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:363:VAL:HG22	1:H:364:PRO:HD2	2.01	0.43
1:A:146:ILE:CG2	1:A:170:THR:HG21	2.49	0.43
1:B:305:ILE:HG13	1:B:305:ILE:O	2.18	0.43
1:E:233:THR:HG21	1:E:235:MET:O	2.19	0.42
1:G:35:LEU:HD23	1:G:116:ILE:HG23	2.01	0.42
1:G:271:ARG:HG2	1:G:271:ARG:HH11	1.84	0.42
1:F:217:ASP:N	1:F:217:ASP:OD1	2.52	0.42
1:B:423:GLY:O	1:B:424:LEU:CB	2.67	0.42
1:C:184:ARG:HH21	1:C:217:ASP:CG	2.26	0.42
1:C:284:LEU:N	1:C:284:LEU:CD1	2.82	0.42
1:C:292:ASP:OD1	1:D:342:ARG:NH2	2.46	0.42
1:D:51:LEU:N	1:D:51:LEU:CD1	2.82	0.42
1:D:332:GLY:O	1:D:333:GLN:C	2.59	0.42
1:H:316:GLN:HG2	1:H:376:ARG:HB3	2.01	0.42
1:B:101:VAL:HB	1:B:102:PRO:HD3	2.01	0.42
1:B:189:GLU:HG3	1:D:365:PHE:CZ	2.55	0.42
1:C:260:LYS:HE3	1:C:280:PRO:O	2.19	0.42
1:C:355:THR:HA	1:C:359:GLN:O	2.19	0.42
1:E:332:GLY:O	1:E:333:GLN:C	2.62	0.42
1:G:209:GLN:HG3	1:G:336:PHE:CG	2.55	0.42
1:F:54:LEU:O	1:F:55:LEU:C	2.63	0.42
1:F:146:ILE:HG23	1:F:170:THR:HG21	2.01	0.42
1:A:209:GLN:HB2	1:A:233:THR:HA	2.02	0.42
1:F:209:GLN:HG2	1:F:336:PHE:CG	2.54	0.42
1:A:217:ASP:OD1	1:A:217:ASP:N	2.53	0.42
1:B:29:ALA:HB3	1:B:132:VAL:HG21	2.01	0.42
1:C:260:LYS:HE2	1:C:280:PRO:O	2.20	0.42
1:D:29:ALA:HB3	1:D:132:VAL:HG21	2.01	0.42
1:G:394:ARG:HH11	1:G:394:ARG:CG	2.31	0.42
1:F:279:ASN:OD1	1:F:281:LEU:HB3	2.20	0.42
1:H:103:TRP:CE3	1:H:107:ARG:NH2	2.88	0.42
1:D:191:GLU:HA	1:D:194:ILE:CG2	2.50	0.42
1:E:215:ILE:HD11	1:E:351:ALA:CB	2.49	0.42
1:G:279:ASN:OD1	1:G:279:ASN:C	2.60	0.42
1:C:279:ASN:C	1:C:279:ASN:OD1	2.63	0.42
1:E:293:PRO:HG2	1:G:338:ARG:HH12	1.85	0.42
1:F:181:GLU:HG2	1:F:269:SER:HA	2.02	0.42
1:H:284:LEU:N	1:H:284:LEU:CD1	2.82	0.42
1:H:355:THR:HA	1:H:359:GLN:O	2.19	0.42
1:H:384:THR:CG2	1:H:406:ILE:HG23	2.50	0.42
1:A:93:TYR:HE1	1:A:329:GLY:HA2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:THR:OG1	1:B:34:PRO:HD3	2.20	0.42
1:B:232:HIS:O	1:B:302:MET:HE1	2.19	0.42
1:C:186:GLY:O	1:C:187:PHE:CB	2.67	0.42
1:D:35:LEU:HD23	1:D:116:ILE:HG23	2.02	0.42
1:E:207:THR:HG22	1:E:254:LYS:HG2	2.01	0.42
1:E:306:ASN:O	1:E:350:ILE:HA	2.20	0.42
1:G:24:PHE:O	1:G:115:ALA:HA	2.19	0.42
1:G:257:HIS:CE1	1:G:289:TYR:OH	2.64	0.42
1:F:19:SER:HB3	1:F:47:GLU:HG2	2.02	0.42
1:F:332:GLY:O	1:F:333:GLN:C	2.61	0.42
1:H:101:VAL:HB	1:H:102:PRO:HD3	2.02	0.42
1:H:408:HIS:NE2	1:G:420:TRP:O	2.41	0.42
1:A:417:GLN:HE22	1:E:145:PRO:CD	2.32	0.42
1:B:24:PHE:CD2	1:B:24:PHE:C	2.98	0.42
1:B:209:GLN:HG3	1:B:336:PHE:CG	2.55	0.42
1:B:312:ASP:CG	1:B:314:THR:HG22	2.44	0.42
1:B:397:ARG:HG2	1:B:398:GLU:N	2.35	0.42
1:C:68:GLU:CD	1:C:90:ARG:HD2	2.45	0.42
1:E:54:LEU:O	1:E:55:LEU:C	2.63	0.42
1:E:333:GLN:HE21	1:E:373:VAL:HG22	1.84	0.42
1:F:306:ASN:O	1:F:350:ILE:HA	2.20	0.41
1:H:352:LEU:O	1:H:352:LEU:HG	2.20	0.41
1:A:332:GLY:O	1:A:333:GLN:C	2.62	0.41
1:C:36:LEU:HG	1:C:62:PHE:HE2	1.85	0.41
1:F:338:ARG:NH1	1:H:338:ARG:HD2	2.35	0.41
1:H:209:GLN:HE21	1:H:336:PHE:HB3	1.84	0.41
1:B:19:SER:OG	1:B:47:GLU:HG3	2.19	0.41
1:B:355:THR:HA	1:B:359:GLN:O	2.18	0.41
1:G:384:THR:HG23	1:G:406:ILE:HG23	2.02	0.41
1:G:385:GLU:OE2	1:G:386:TRP:CZ3	2.73	0.41
1:F:294:PHE:CE2	1:H:294:PHE:HB2	2.55	0.41
1:F:355:THR:HA	1:F:359:GLN:O	2.20	0.41
1:H:189:GLU:OE1	1:H:192:ARG:NH1	2.53	0.41
1:A:101:VAL:HB	1:A:102:PRO:HD3	2.02	0.41
1:B:216:PRO:HG3	1:B:305:ILE:HD11	2.02	0.41
1:B:248:LEU:HD12	1:B:248:LEU:HA	1.91	0.41
1:G:43:LYS:HB2	1:G:67:MET:CE	2.50	0.41
1:H:24:PHE:O	1:H:115:ALA:HA	2.21	0.41
1:H:35:LEU:HD23	1:H:116:ILE:HG23	2.02	0.41
1:A:54:LEU:O	1:A:55:LEU:C	2.63	0.41
1:C:342:ARG:NH1	2:C:502:HOH:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:GLN:HG3	1:D:336:PHE:CG	2.54	0.41
1:E:279:ASN:OD1	1:E:279:ASN:C	2.63	0.41
1:G:382:VAL:HG23	1:G:391:LEU:HD22	2.01	0.41
1:A:355:THR:HA	1:A:359:GLN:O	2.21	0.41
1:D:284:LEU:CD1	1:D:284:LEU:N	2.83	0.41
1:E:384:THR:HG23	1:E:406:ILE:HD12	2.02	0.41
1:A:203:GLU:HG3	1:A:301:LYS:HE3	2.02	0.41
1:C:6:LYS:HD2	1:C:169:PHE:O	2.20	0.41
1:C:32:PRO:CB	1:C:150:MET:HE3	2.50	0.41
1:C:63:ALA:HA	1:C:90:ARG:HH22	1.83	0.41
1:C:209:GLN:HB2	1:C:233:THR:HA	2.02	0.41
1:A:34:PRO:HD2	1:A:150:MET:CE	2.47	0.41
1:E:215:ILE:CD1	1:E:351:ALA:HB1	2.50	0.41
1:E:382:VAL:HG23	1:E:391:LEU:CD2	2.51	0.41
1:A:98:LEU:HD11	1:A:135:ILE:CG2	2.50	0.41
1:C:217:ASP:OD1	1:C:217:ASP:N	2.53	0.41
1:E:285:HIS:HB2	1:E:290:VAL:HG23	2.03	0.41
1:E:294[A]:PHE:CD1	1:G:294:PHE:CE2	3.08	0.41
1:G:96:VAL:O	1:G:96:VAL:HG13	2.20	0.41
1:H:53:HIS:HD2	1:H:54:LEU:O	2.03	0.41
1:H:209:GLN:HG3	1:H:336:PHE:CG	2.56	0.41
1:A:24:PHE:CD2	1:A:24:PHE:C	2.99	0.41
1:A:54:LEU:HD13	1:A:76:LEU:HB2	2.03	0.41
1:A:194:ILE:HG12	1:A:384:THR:C	2.46	0.41
1:A:257:HIS:CD2	1:A:283:GLU:OE2	2.74	0.41
1:B:152:ASN:HA	1:B:153:PRO:HD2	1.92	0.41
1:B:158:THR:HG22	1:B:276:VAL:HG13	2.03	0.41
1:B:226:ARG:HH11	1:B:226:ARG:CG	2.33	0.41
1:B:236:ILE:HB	1:B:266:VAL:HG22	2.02	0.41
1:B:285:HIS:HB2	1:B:290:VAL:HG23	2.02	0.41
1:C:22:ARG:HD2	1:C:111:PRO:O	2.21	0.41
1:C:24:PHE:O	1:C:115:ALA:HA	2.19	0.41
1:D:216:PRO:HG3	1:D:305:ILE:HD11	2.02	0.41
1:D:384:THR:HG23	1:D:406:ILE:HG22	2.01	0.41
1:E:194:ILE:HG12	1:E:384:THR:C	2.46	0.41
1:E:383:VAL:HG22	1:E:388:VAL:HG22	2.03	0.41
1:G:233:THR:HG22	1:G:235:MET:H	1.85	0.41
1:H:332:GLY:O	1:H:333:GLN:C	2.62	0.41
1:A:88[B]:GLN:NE2	1:A:90:ARG:HG3	2.36	0.41
1:A:257:HIS:CE1	1:A:289:TYR:OH	2.64	0.41
1:B:204:ASP:OD2	1:B:226:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ILE:HG23	1:B:381:TYR:O	2.21	0.41
1:G:24:PHE:CD2	1:G:24:PHE:C	2.99	0.41
1:F:334:LEU:HD13	1:F:338:ARG:NH1	2.37	0.40
1:H:53:HIS:CD2	1:H:56:GLN:HG3	2.56	0.40
1:B:44:ASP:OD1	1:B:44:ASP:N	2.50	0.40
1:C:101:VAL:HB	1:C:102:PRO:HD3	2.03	0.40
1:C:256:LEU:HG	1:C:257:HIS:ND1	2.36	0.40
1:E:25:VAL:HG11	1:E:36:LEU:HD21	2.02	0.40
1:G:191:GLU:HA	1:G:194:ILE:CG2	2.51	0.40
1:H:285:HIS:HB2	1:H:290:VAL:HG23	2.03	0.40
1:B:54:LEU:O	1:B:55:LEU:C	2.62	0.40
1:F:35:LEU:HD23	1:F:116:ILE:HG23	2.03	0.40
1:F:417:GLN:OE1	1:C:145:PRO:CD	2.69	0.40
1:B:11:GLU:CD	1:B:11:GLU:H	2.29	0.40
1:C:194:ILE:HG12	1:C:384:THR:C	2.46	0.40
1:D:191:GLU:O	1:D:194:ILE:HG23	2.22	0.40
1:G:355:THR:HA	1:G:359:GLN:O	2.20	0.40
1:H:306:ASN:O	1:H:350:ILE:HA	2.22	0.40
1:B:306:ASN:O	1:B:350:ILE:HA	2.21	0.40
1:B:363:VAL:HG22	1:B:364:PRO:HD2	2.03	0.40
1:C:353:PRO:O	1:C:361:ARG:HD2	2.21	0.40
1:D:257:HIS:CD2	1:D:283:GLU:OE2	2.74	0.40
1:D:425:LEU:O	1:D:427:ARG:N	2.55	0.40
1:E:72:ARG:NH2	1:G:397:ARG:NH2	2.69	0.40
1:E:257:HIS:O	1:E:260:LYS:HB2	2.22	0.40
1:E:279:ASN:OD1	1:E:281:LEU:HB3	2.22	0.40
1:G:260:LYS:HE2	1:G:280:PRO:O	2.21	0.40
1:C:285:HIS:HB2	1:C:290:VAL:HG23	2.04	0.40
1:E:36:LEU:HD12	1:E:36:LEU:HA	1.99	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	427/450 (95%)	392 (92%)	29 (7%)	6 (1%)	9	12
1	B	420/450 (93%)	378 (90%)	37 (9%)	5 (1%)	10	15
1	C	422/450 (94%)	385 (91%)	29 (7%)	8 (2%)	6	8
1	D	421/450 (94%)	382 (91%)	33 (8%)	6 (1%)	9	12
1	E	420/450 (93%)	383 (91%)	31 (7%)	6 (1%)	9	12
1	F	420/450 (93%)	383 (91%)	31 (7%)	6 (1%)	9	12
1	G	422/450 (94%)	382 (90%)	32 (8%)	8 (2%)	6	8
1	H	421/450 (94%)	383 (91%)	31 (7%)	7 (2%)	7	9
All	All	3373/3600 (94%)	3068 (91%)	253 (8%)	52 (2%)	8	11

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	135	ILE
1	F	323	GLY
1	H	55	LEU
1	H	56	GLN
1	H	135	ILE
1	A	135	ILE
1	A	323	GLY
1	B	135	ILE
1	B	424	LEU
1	C	63	ALA
1	C	135	ILE
1	C	187	PHE
1	C	323	GLY
1	C	424	LEU
1	D	135	ILE
1	E	59	GLU
1	E	60	ASP
1	E	135	ILE
1	G	55	LEU
1	G	64	SER
1	G	135	ILE
1	G	212	ILE
1	G	323	GLY
1	F	15	GLY
1	H	15	GLY
1	H	211	GLY
1	H	323	GLY

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Mol	Chain	Res	Type
1	A	15	GLY
1	B	15	GLY
1	B	323	GLY
1	C	15	GLY
1	C	211	GLY
1	D	15	GLY
1	D	52	VAL
1	D	323	GLY
1	E	15	GLY
1	E	211	GLY
1	G	15	GLY
1	G	56	GLN
1	G	174	GLU
1	F	187	PHE
1	H	4	ARG
1	A	426	PRO
1	D	426	PRO
1	F	147	VAL
1	B	211	GLY
1	D	211	GLY
1	A	147	VAL
1	A	211	GLY
1	C	147	VAL
1	E	147	VAL
1	F	211	GLY

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	337/362 (93%)	280 (83%)	57 (17%)	2	2
1	B	328/362 (91%)	270 (82%)	58 (18%)	2	2
1	C	333/362 (92%)	277 (83%)	56 (17%)	2	2
1	D	333/362 (92%)	272 (82%)	61 (18%)	2	1
1	E	327/362 (90%)	274 (84%)	53 (16%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	333/362 (92%)	280 (84%)	53 (16%)	2	2
1	G	330/362 (91%)	264 (80%)	66 (20%)	1	1
1	H	329/362 (91%)	272 (83%)	57 (17%)	2	2
All	All	2650/2896 (92%)	2189 (83%)	461 (17%)	2	2

All (461) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	8	THR
1	F	12	ASP
1	F	14	VAL
1	F	16	LEU
1	F	18	ARG
1	F	36	LEU
1	F	51	LEU
1	F	54	LEU
1	F	75	SER
1	F	83	ARG
1	F	84	GLU
1	F	88	GLN
1	F	96	VAL
1	F	104	LEU
1	F	107	ARG
1	F	110	LEU
1	F	117	VAL
1	F	119	VAL
1	F	132	VAL
1	F	135	ILE
1	F	146	ILE
1	F	151	VAL
1	F	166	VAL
1	F	168	ARG
1	F	183	LYS
1	F	192	ARG
1	F	201	LEU
1	F	210	MET
1	F	216	PRO
1	F	223	LEU
1	F	226	ARG
1	F	229	LEU
1	F	236	ILE

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Mol	Chain	Res	Type
1	F	248	LEU
1	F	264	THR
1	F	270	GLU
1	F	274	ARG
1	F	303	VAL
1	F	313	LEU
1	F	314	THR
1	F	322	ILE
1	F	324	THR
1	F	334	LEU
1	F	344	GLU
1	F	352	LEU
1	F	366	LEU
1	F	373	VAL
1	F	379	VAL
1	F	391	LEU
1	F	397	ARG
1	F	416	LEU
1	F	422	ARG
1	F	424	LEU
1	H	8	THR
1	H	11	GLU
1	H	14	VAL
1	H	16	LEU
1	H	39	LEU
1	H	44	ASP
1	H	52	VAL
1	H	65	LEU
1	H	66	GLU
1	H	67	MET
1	H	72	ARG
1	H	75	SER
1	H	76	LEU
1	H	80	PRO
1	H	94	VAL
1	H	104	LEU
1	H	130	LEU
1	H	135	ILE
1	H	142	GLU
1	H	145	PRO
1	H	168	ARG
1	H	184	ARG

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Mol	Chain	Res	Type
1	H	185	GLU
1	H	191	GLU
1	H	194	ILE
1	H	201	LEU
1	H	207	THR
1	H	208	LEU
1	H	212	ILE
1	H	216	PRO
1	H	220	LEU
1	H	223	LEU
1	H	226	ARG
1	H	227	ARG
1	H	229	LEU
1	H	248	LEU
1	H	270	GLU
1	H	274	ARG
1	H	281	LEU
1	H	295	VAL
1	H	296	ILE
1	H	300	ARG
1	H	303	VAL
1	H	305	ILE
1	H	313	LEU
1	H	314	THR
1	H	324	THR
1	H	357	LYS
1	H	362	ILE
1	H	379	VAL
1	H	391	LEU
1	H	394	ARG
1	H	403	LEU
1	H	406	ILE
1	H	416	LEU
1	H	420	TRP
1	H	421	GLU
1	A	7	LEU
1	A	8	THR
1	A	14	VAL
1	A	16	LEU
1	A	36	LEU
1	A	43	LYS
1	A	47	GLU

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Mol	Chain	Res	Type
1	A	51	LEU
1	A	59	GLU
1	A	75	SER
1	A	88[A]	GLN
1	A	88[B]	GLN
1	A	96	VAL
1	A	98	LEU
1	A	104	LEU
1	A	110	LEU
1	A	119	VAL
1	A	132	VAL
1	A	135	ILE
1	A	146	ILE
1	A	147	VAL
1	A	151	VAL
1	A	166	VAL
1	A	168	ARG
1	A	183	LYS
1	A	189	GLU
1	A	201	LEU
1	A	207	THR
1	A	208	LEU
1	A	210	MET
1	A	216	PRO
1	A	223	LEU
1	A	224	GLU
1	A	226	ARG
1	A	229	LEU
1	A	246	LYS
1	A	248	LEU
1	A	270	GLU
1	A	271	ARG
1	A	284	LEU
1	A	303	VAL
1	A	313	LEU
1	A	322	ILE
1	A	324	THR
1	A	334	LEU
1	A	352	LEU
1	A	359	GLN
1	A	366	LEU
1	A	373	VAL

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Mol	Chain	Res	Type
1	A	374	THR
1	A	379	VAL
1	A	391	LEU
1	A	401	LYS
1	A	416	LEU
1	A	421	GLU
1	A	422	ARG
1	A	424	LEU
1	B	7	LEU
1	B	8	THR
1	B	11	GLU
1	B	14	VAL
1	B	21	MET
1	B	39	LEU
1	B	44	ASP
1	B	47	GLU
1	B	52	VAL
1	B	57	MET
1	B	59	GLU
1	B	67	MET
1	B	72	ARG
1	B	80	PRO
1	B	83	ARG
1	B	94	VAL
1	B	98	LEU
1	B	104	LEU
1	B	130	LEU
1	B	135	ILE
1	B	142	GLU
1	B	145	PRO
1	B	151	VAL
1	B	184	ARG
1	B	191	GLU
1	B	194	ILE
1	B	196	GLU
1	B	201	LEU
1	B	207	THR
1	B	208	LEU
1	B	216	PRO
1	B	220	LEU
1	B	223	LEU
1	B	224	GLU

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Mol	Chain	Res	Type
1	B	226	ARG
1	B	227	ARG
1	B	229	LEU
1	B	248	LEU
1	B	281	LEU
1	B	295	VAL
1	B	296	ILE
1	B	300	ARG
1	B	305	ILE
1	B	313	LEU
1	B	314	THR
1	B	324	THR
1	B	343	SER
1	B	350	ILE
1	B	352	LEU
1	B	357	LYS
1	B	362	ILE
1	B	379	VAL
1	B	391	LEU
1	B	396	LEU
1	B	397	ARG
1	B	406	ILE
1	B	413	GLU
1	B	416	LEU
1	C	8	THR
1	C	14	VAL
1	C	36	LEU
1	C	43	LYS
1	C	47	GLU
1	C	51	LEU
1	C	54	LEU
1	C	64	SER
1	C	75	SER
1	C	80	PRO
1	C	96	VAL
1	C	104	LEU
1	C	110	LEU
1	C	119	VAL
1	C	124	GLU
1	C	132	VAL
1	C	135	ILE
1	C	146	ILE

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Mol	Chain	Res	Type
1	C	147	VAL
1	C	151	VAL
1	C	166	VAL
1	C	168	ARG
1	C	185	GLU
1	C	187	PHE
1	C	192	ARG
1	C	201	LEU
1	C	208	LEU
1	C	215	ILE
1	C	216	PRO
1	C	217	ASP
1	C	220	LEU
1	C	223	LEU
1	C	224	GLU
1	C	229	LEU
1	C	235	MET
1	C	236	ILE
1	C	246	LYS
1	C	264	THR
1	C	270	GLU
1	C	301	LYS
1	C	303	VAL
1	C	313	LEU
1	C	314	THR
1	C	322	ILE
1	C	324	THR
1	C	334	LEU
1	C	342	ARG
1	C	352	LEU
1	C	366	LEU
1	C	373	VAL
1	C	379	VAL
1	C	391	LEU
1	C	413	GLU
1	C	416	LEU
1	C	421	GLU
1	C	422	ARG
1	D	6	LYS
1	D	7	LEU
1	D	8	THR
1	D	14	VAL

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Mol	Chain	Res	Type
1	D	16	LEU
1	D	25	VAL
1	D	39	LEU
1	D	43	LYS
1	D	51	LEU
1	D	52	VAL
1	D	64	SER
1	D	65	LEU
1	D	67	MET
1	D	72	ARG
1	D	80	PRO
1	D	83	ARG
1	D	84	GLU
1	D	94	VAL
1	D	104	LEU
1	D	130	LEU
1	D	135	ILE
1	D	142	GLU
1	D	145	PRO
1	D	151	VAL
1	D	167	SER
1	D	183	LYS
1	D	189	GLU
1	D	191	GLU
1	D	194	ILE
1	D	201	LEU
1	D	207	THR
1	D	208	LEU
1	D	220	LEU
1	D	223	LEU
1	D	226	ARG
1	D	229	LEU
1	D	248	LEU
1	D	249	ILE
1	D	270	GLU
1	D	281	LEU
1	D	295	VAL
1	D	300	ARG
1	D	305	ILE
1	D	313	LEU
1	D	314	THR
1	D	322	ILE

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Mol	Chain	Res	Type
1	D	324	THR
1	D	325	ARG
1	D	342	ARG
1	D	357	LYS
1	D	361	ARG
1	D	363	VAL
1	D	379	VAL
1	D	391	LEU
1	D	394	ARG
1	D	396	LEU
1	D	401	LYS
1	D	413	GLU
1	D	416	LEU
1	D	417	GLN
1	D	424	LEU
1	E	7	LEU
1	E	8	THR
1	E	14	VAL
1	E	36	LEU
1	E	42	ARG
1	E	43	LYS
1	E	51	LEU
1	E	54	LEU
1	E	64	SER
1	E	75	SER
1	E	80	PRO
1	E	83	ARG
1	E	104	LEU
1	E	110	LEU
1	E	117	VAL
1	E	119	VAL
1	E	124	GLU
1	E	132	VAL
1	E	135	ILE
1	E	147	VAL
1	E	166	VAL
1	E	168	ARG
1	E	184	ARG
1	E	185	GLU
1	E	192	ARG
1	E	208	LEU
1	E	215	ILE

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Mol	Chain	Res	Type
1	E	216	PRO
1	E	223	LEU
1	E	226	ARG
1	E	229	LEU
1	E	235	MET
1	E	248	LEU
1	E	264	THR
1	E	270	GLU
1	E	284	LEU
1	E	303	VAL
1	E	313	LEU
1	E	314	THR
1	E	322	ILE
1	E	324	THR
1	E	333	GLN
1	E	334	LEU
1	E	344	GLU
1	E	352	LEU
1	E	366	LEU
1	E	373	VAL
1	E	374	THR
1	E	379	VAL
1	E	391	LEU
1	E	397	ARG
1	E	416	LEU
1	E	420	TRP
1	G	8	THR
1	G	11	GLU
1	G	14	VAL
1	G	16	LEU
1	G	33	THR
1	G	39	LEU
1	G	46	LEU
1	G	52	VAL
1	G	56	GLN
1	G	57	MET
1	G	59	GLU
1	G	65	LEU
1	G	66	GLU
1	G	67	MET
1	G	68	GLU
1	G	72	ARG

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Mol	Chain	Res	Type
1	G	75	SER
1	G	83	ARG
1	G	90	ARG
1	G	94	VAL
1	G	98	LEU
1	G	104	LEU
1	G	130	LEU
1	G	135	ILE
1	G	142	GLU
1	G	143	THR
1	G	151	VAL
1	G	168	ARG
1	G	174	GLU
1	G	184	ARG
1	G	185	GLU
1	G	189	GLU
1	G	191	GLU
1	G	194	ILE
1	G	201	LEU
1	G	207	THR
1	G	208	LEU
1	G	215	ILE
1	G	216	PRO
1	G	220	LEU
1	G	223	LEU
1	G	226	ARG
1	G	229	LEU
1	G	248	LEU
1	G	255	SER
1	G	270	GLU
1	G	281	LEU
1	G	295	VAL
1	G	296	ILE
1	G	305	ILE
1	G	313	LEU
1	G	322	ILE
1	G	324	THR
1	G	357	LYS
1	G	362	ILE
1	G	376	ARG
1	G	379	VAL
1	G	391	LEU

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Mol	Chain	Res	Type
1	G	394	ARG
1	G	396	LEU
1	G	397	ARG
1	G	406	ILE
1	G	416	LEU
1	G	422	ARG
1	G	424	LEU
1	G	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	56	GLN
1	F	118	GLN
1	F	209	GLN
1	F	232	HIS
1	F	257	HIS
1	F	285	HIS
1	F	291	ASN
1	F	298	GLN
1	F	299	ASN
1	F	306	ASN
1	F	316	GLN
1	F	333	GLN
1	H	53	HIS
1	H	118	GLN
1	H	165	HIS
1	H	197	HIS
1	H	209	GLN
1	H	232	HIS
1	H	257	HIS
1	H	298	GLN
1	H	306	ASN
1	H	316	GLN
1	H	380	HIS
1	A	56	GLN
1	A	118	GLN
1	A	209	GLN
1	A	257	HIS
1	A	285	HIS
1	A	298	GLN
1	A	299	ASN

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Mol	Chain	Res	Type
1	A	306	ASN
1	A	316	GLN
1	A	333	GLN
1	A	359	GLN
1	A	417	GLN
1	B	53	HIS
1	B	56	GLN
1	B	88	GLN
1	B	118	GLN
1	B	165	HIS
1	B	209	GLN
1	B	232	HIS
1	B	257	HIS
1	B	298	GLN
1	B	306	ASN
1	B	316	GLN
1	B	333	GLN
1	B	380	HIS
1	C	56	GLN
1	C	118	GLN
1	C	209	GLN
1	C	257	HIS
1	C	285	HIS
1	C	291	ASN
1	C	298	GLN
1	C	299	ASN
1	C	306	ASN
1	C	316	GLN
1	C	333	GLN
1	C	359	GLN
1	C	380	HIS
1	D	118	GLN
1	D	165	HIS
1	D	209	GLN
1	D	232	HIS
1	D	257	HIS
1	D	298	GLN
1	D	306	ASN
1	D	316	GLN
1	D	333	GLN
1	D	380	HIS
1	E	28	ASN

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Mol	Chain	Res	Type
1	E	56	GLN
1	E	118	GLN
1	E	209	GLN
1	E	232	HIS
1	E	257	HIS
1	E	285	HIS
1	E	291	ASN
1	E	298	GLN
1	E	299	ASN
1	E	306	ASN
1	E	316	GLN
1	E	333	GLN
1	G	53	HIS
1	G	56	GLN
1	G	118	GLN
1	G	165	HIS
1	G	197	HIS
1	G	209	GLN
1	G	232	HIS
1	G	257	HIS
1	G	298	GLN
1	G	306	ASN
1	G	316	GLN
1	G	380	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	426/450 (94%)	0.46	13 (3%) 51 45	19, 48, 87, 112	3 (0%)
1	B	422/450 (93%)	0.44	9 (2%) 63 59	25, 47, 82, 124	0
1	C	422/450 (93%)	0.48	12 (2%) 55 50	19, 45, 78, 113	2 (0%)
1	D	423/450 (94%)	0.54	17 (4%) 42 35	27, 48, 86, 119	0
1	E	421/450 (93%)	0.46	20 (4%) 35 29	19, 45, 75, 125	1 (0%)
1	F	422/450 (93%)	0.47	14 (3%) 49 43	21, 48, 78, 117	0
1	G	424/450 (94%)	0.65	23 (5%) 31 26	28, 50, 85, 123	0
1	H	423/450 (94%)	0.50	11 (2%) 57 52	27, 49, 79, 120	0
All	All	3383/3600 (93%)	0.50	119 (3%) 47 41	19, 48, 82, 125	6 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	212	ILE	4.6
1	G	328	SER	4.5
1	F	212	ILE	4.4
1	G	82	ASP	4.3
1	D	212	ILE	4.3
1	B	420	TRP	4.1
1	G	212	ILE	4.1
1	B	212	ILE	4.1
1	A	2	SER	3.9
1	G	319	ALA	3.8
1	E	420	TRP	3.7
1	C	4	ARG	3.6
1	A	4[A]	ARG	3.5
1	D	211	GLY	3.5
1	G	220	LEU	3.3
1	G	4	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	91	ALA	3.3
1	G	215	ILE	3.3
1	D	52	VAL	3.2
1	H	420	TRP	3.2
1	C	88	GLN	3.1
1	B	62	PHE	3.1
1	A	423	GLY	3.0
1	A	3	TYR	3.0
1	G	422	ARG	3.0
1	G	81	ALA	3.0
1	G	339	GLY	3.0
1	G	327	TYR	3.0
1	G	230	GLY	2.9
1	E	424	LEU	2.9
1	F	5	LYS	2.9
1	D	424	LEU	2.9
1	C	187	PHE	2.9
1	F	426	PRO	2.8
1	B	424	LEU	2.8
1	G	77	PHE	2.8
1	F	186	GLY	2.8
1	E	88	GLN	2.7
1	H	425	LEU	2.7
1	G	329	GLY	2.7
1	G	213	GLY	2.7
1	F	36	LEU	2.7
1	D	126	GLY	2.7
1	D	242	GLU	2.7
1	F	8	THR	2.7
1	G	149	ALA	2.7
1	H	194	ILE	2.6
1	A	323	GLY	2.6
1	D	7	LEU	2.6
1	B	328	SER	2.5
1	B	7	LEU	2.5
1	C	423	GLY	2.5
1	D	339	GLY	2.5
1	F	216	PRO	2.5
1	H	65	LEU	2.5
1	E	92	ASP	2.5
1	D	6	LYS	2.5
1	B	4	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	422	ARG	2.4
1	G	65	LEU	2.4
1	E	333	GLN	2.4
1	F	92	ASP	2.4
1	G	5	LYS	2.4
1	C	321	SER	2.3
1	E	215	ILE	2.3
1	G	237	SER	2.3
1	F	423	GLY	2.3
1	E	213	GLY	2.3
1	A	213	GLY	2.3
1	F	78	VAL	2.3
1	C	358	GLY	2.2
1	C	420	TRP	2.2
1	H	40	ALA	2.2
1	F	328	SER	2.2
1	E	186	GLY	2.2
1	E	328	SER	2.2
1	C	366	LEU	2.2
1	A	78	VAL	2.2
1	C	212	ILE	2.2
1	E	294[A]	PHE	2.2
1	H	81	ALA	2.2
1	C	356	ALA	2.2
1	E	342	ARG	2.2
1	C	327	TYR	2.2
1	D	5	LYS	2.2
1	A	117	VAL	2.2
1	D	210	MET	2.2
1	A	427	ARG	2.2
1	F	322	ILE	2.2
1	G	78	VAL	2.2
1	E	13	ALA	2.1
1	E	187	PHE	2.1
1	G	330	PHE	2.1
1	D	327	TYR	2.1
1	H	328	SER	2.1
1	H	184	ARG	2.1
1	D	162	THR	2.1
1	A	7	LEU	2.1
1	B	220	LEU	2.1
1	H	288	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	77	PHE	2.1
1	C	80	PRO	2.1
1	D	333	GLN	2.1
1	E	366	LEU	2.1
1	A	329	GLY	2.1
1	F	327	TYR	2.1
1	A	44	ASP	2.0
1	H	64	SER	2.0
1	D	91	ALA	2.0
1	G	80	PRO	2.0
1	G	210	MET	2.0
1	E	54	LEU	2.0
1	E	65	LEU	2.0
1	E	397	ARG	2.0
1	A	85	ALA	2.0
1	B	6	LYS	2.0
1	E	8	THR	2.0
1	F	211	GLY	2.0
1	E	212	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.