



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:50 AM UTC

PDB ID : 3PVA / pdb_00003pva
Title : PENICILLIN V ACYLASE FROM B. SPHAERICUS
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Mcvey, C.E.; Verma, C.S.; Dauter, Z.; Dodson, E.J.; Dodson, G.G.
Deposited on : 1998-11-13
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

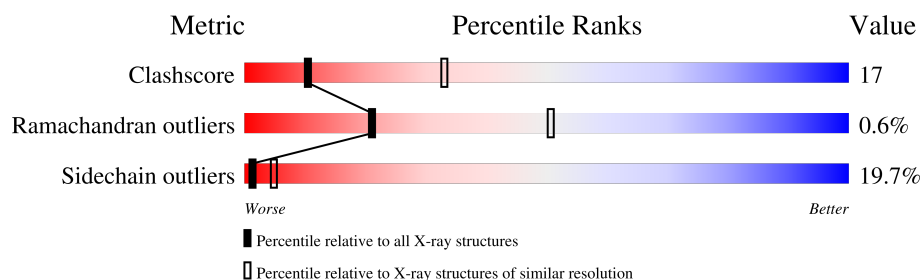
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	59% 29% 10% .
1	B	335	58% 30% 10% .
1	C	335	56% 32% 10% .
1	D	335	58% 30% 10% .
1	E	335	55% 33% 10% .
1	F	335	53% 34% 10% .
1	G	335	57% 31% 10% .
1	H	335	54% 33% 11% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23640 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 PROTEIN (PENICILLIN V ACYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2605	1658	425	508	14			
1	B	334	Total	C	N	O	S	0	0	0
			2605	1658	425	508	14			
1	C	334	Total	C	N	O	S	0	0	0
			2605	1658	425	508	14			
1	D	334	Total	C	N	O	S	0	0	0
			2605	1658	425	508	14			
1	E	334	Total	C	N	O	S	0	0	0
			2605	1658	425	508	14			
1	F	334	Total	C	N	O	S	0	0	0
			2605	1658	425	508	14			
1	G	334	Total	C	N	O	S	0	0	0
			2605	1658	425	508	14			
1	H	334	Total	C	N	O	S	0	0	0
			2605	1658	425	508	14			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	346	Total	O	0	0
			346	346		
2	B	348	Total	O	0	0
			348	348		
2	C	350	Total	O	0	0
			350	350		
2	D	356	Total	O	0	0
			356	356		
2	E	353	Total	O	0	0
			353	353		
2	F	350	Total	O	0	0
			350	350		

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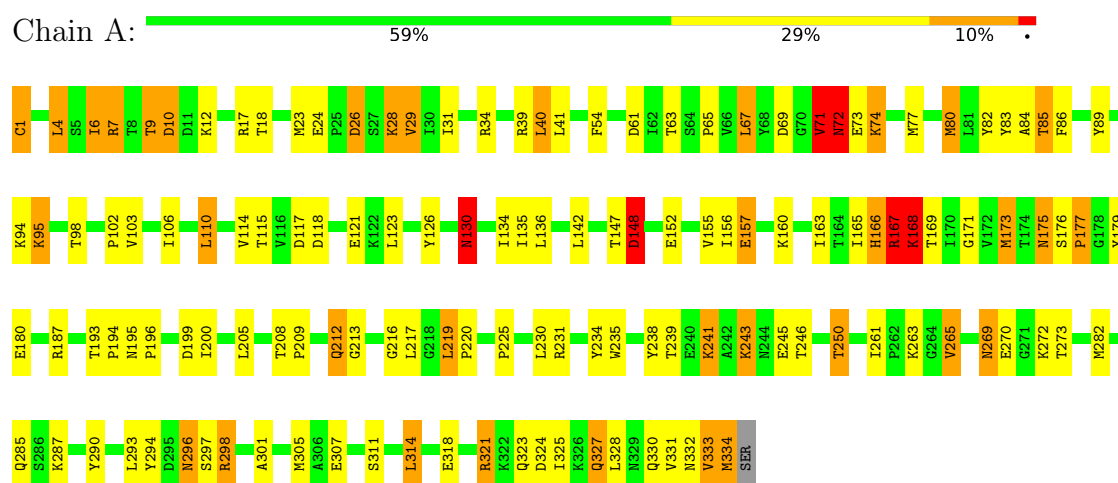
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	351	Total 351	O 351	0	0
2	H	346	Total 346	O 346	0	0

3 Residue-property plots [i](#)

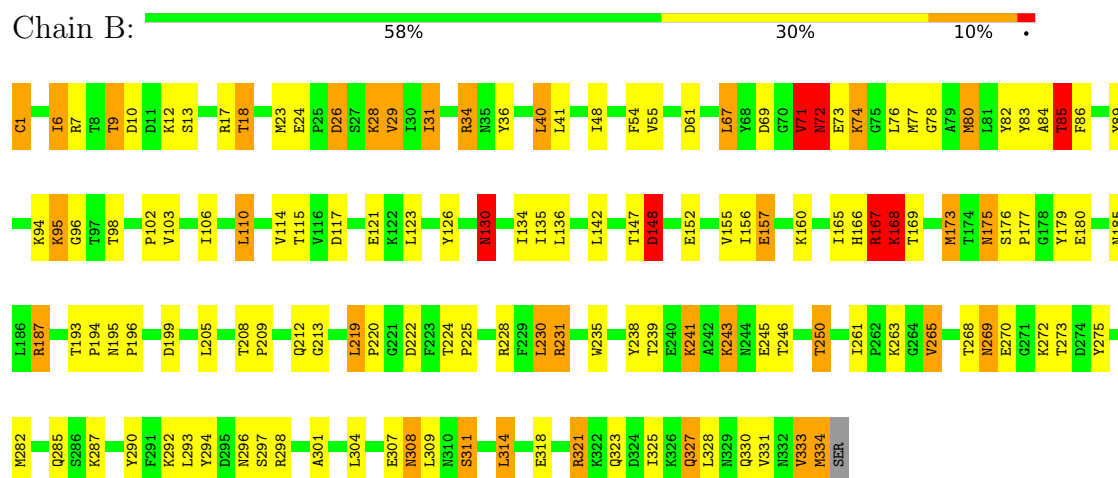
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

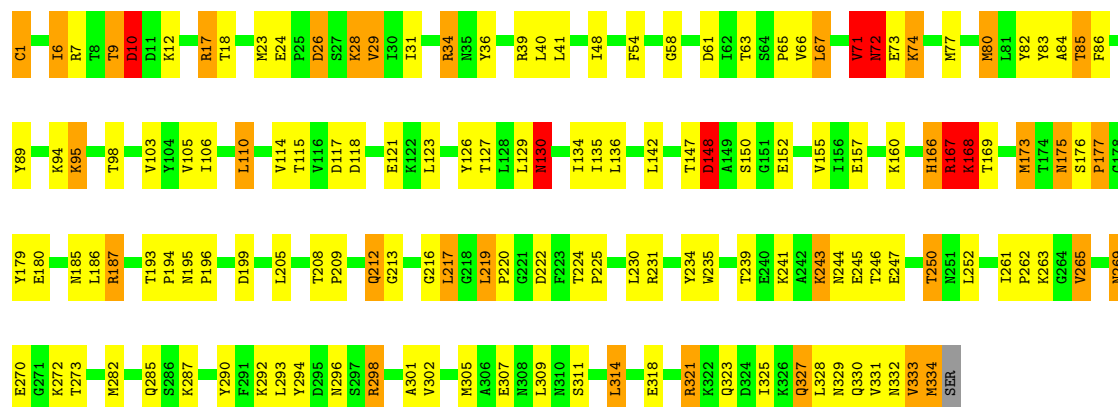


• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)



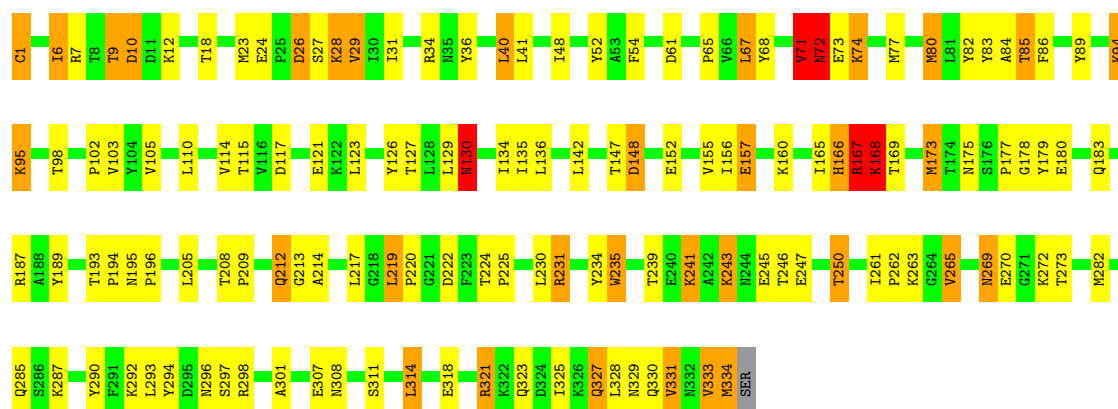
• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)





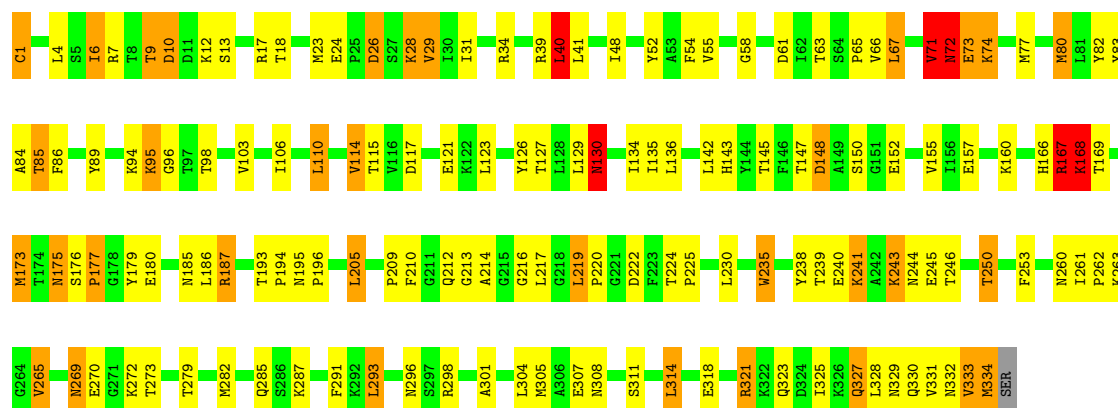
• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain D: 58% 30% 10% .



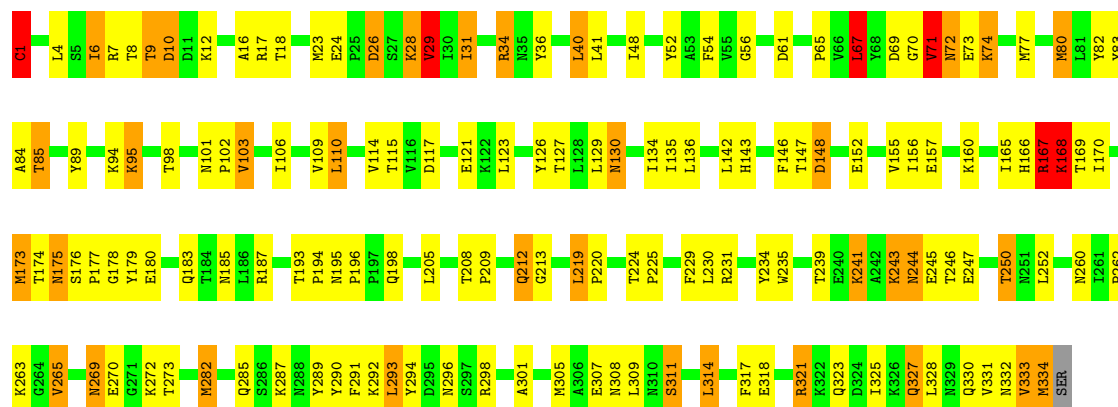
• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain E: 55% 33% 10% .



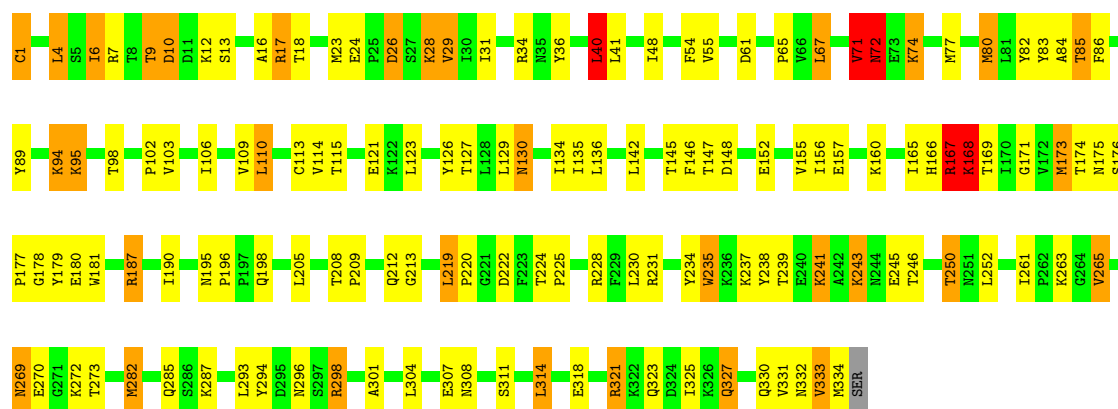
• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain F: 53% 34% 10% .



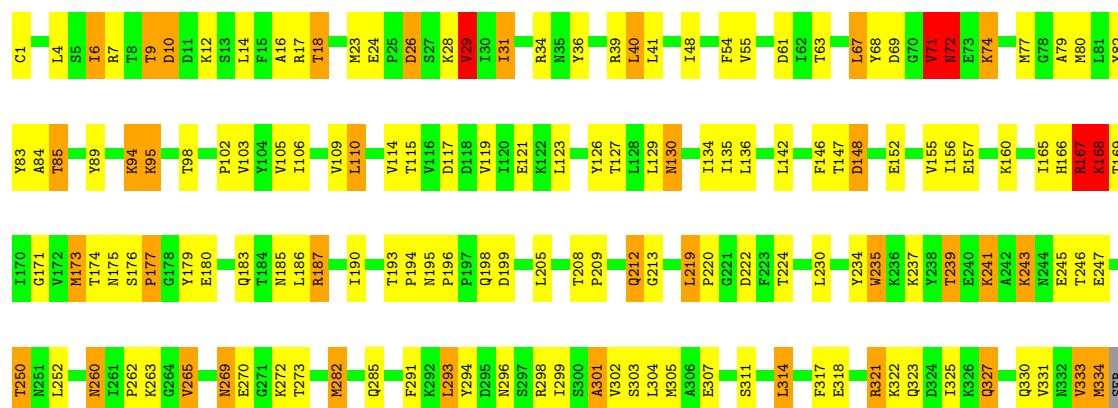
• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain G: 57% 31% 10%



• Molecule 1: PROTEIN (PENICILLIN V ACYLASE)

Chain H: 54% 33% 11%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.40 Å 129.60 Å 156.70 Å 88.30° 83.40° 84.60°	Depositor
Resolution (Å)	14.00 – 2.80	Depositor
% Data completeness (in resolution range)	85.0 (14.00-2.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23640	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

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	0.63	0/2660	1.61	45/3617 (1.2%)
1	B	0.67	0/2660	1.63	42/3617 (1.2%)
1	C	0.64	0/2660	1.61	45/3617 (1.2%)
1	D	0.64	0/2660	1.62	48/3617 (1.3%)
1	E	0.62	0/2660	1.64	45/3617 (1.2%)
1	F	0.61	0/2660	1.61	40/3617 (1.1%)
1	G	0.65	0/2660	1.62	43/3617 (1.2%)
1	H	0.62	0/2660	1.61	39/3617 (1.1%)
All	All	0.63	0/21280	1.62	347/28936 (1.2%)

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	2
1	B	0	2
1	C	0	2
1	E	0	3
1	G	0	1
1	H	0	1
All	All	0	11

There are no bond length outliers.

All (347) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	261	ILE	N-CA-C	10.87	117.45	107.56
1	E	261	ILE	N-CA-C	9.79	116.47	107.56
1	B	85	THR	N-CA-CB	-9.74	103.06	114.17
1	D	72	ASN	CB-CA-C	-9.52	93.99	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	71	VAL	CB-CA-C	-9.21	97.63	110.90
1	C	261	ILE	N-CA-C	9.18	115.92	107.56
1	B	9	THR	CA-C-N	9.12	139.36	121.58
1	B	9	THR	C-N-CA	9.12	139.36	121.58
1	C	71	VAL	CB-CA-C	-9.00	97.94	110.90
1	E	296	ASN	CA-CB-CG	8.89	121.49	112.60
1	F	213	GLY	N-CA-C	8.42	125.10	115.08
1	D	261	ILE	N-CA-C	8.34	116.18	107.76
1	A	177	PRO	CA-C-N	8.33	128.01	120.10
1	A	177	PRO	C-N-CA	8.33	128.01	120.10
1	A	261	ILE	N-CA-C	8.27	115.09	107.56
1	A	167	ARG	CD-NE-CZ	8.20	135.88	124.40
1	H	72	ASN	CB-CA-C	-8.19	95.02	110.51
1	D	71	VAL	CB-CA-C	-8.08	99.27	110.90
1	E	177	PRO	CA-C-N	8.07	127.77	120.10
1	E	177	PRO	C-N-CA	8.07	127.77	120.10
1	F	117	ASP	CA-CB-CG	-8.03	104.57	112.60
1	G	72	ASN	CB-CA-C	-8.02	95.35	110.51
1	D	9	THR	CA-C-N	8.00	137.17	121.58
1	D	9	THR	C-N-CA	8.00	137.17	121.58
1	E	269	ASN	CA-C-O	7.95	128.84	120.42
1	H	195	ASN	N-CA-C	7.89	120.01	110.07
1	B	213	GLY	N-CA-C	7.88	124.07	114.69
1	H	10	ASP	CA-CB-CG	7.88	120.48	112.60
1	E	167	ARG	CD-NE-CZ	7.83	135.36	124.40
1	C	72	ASN	CB-CA-C	-7.81	95.76	110.51
1	E	213	GLY	N-CA-C	7.75	123.91	114.69
1	D	217	LEU	CA-C-O	-7.73	112.45	120.80
1	C	167	ARG	CD-NE-CZ	7.71	135.20	124.40
1	A	213	GLY	N-CA-C	7.71	124.25	115.08
1	B	167	ARG	CD-NE-CZ	7.70	135.18	124.40
1	A	72	ASN	CB-CA-C	-7.62	96.10	110.51
1	C	9	THR	CA-C-N	7.58	136.35	121.58
1	C	9	THR	C-N-CA	7.58	136.35	121.58
1	G	167	ARG	CD-NE-CZ	7.56	134.99	124.40
1	F	195	ASN	N-CA-C	7.56	119.59	110.07
1	H	187	ARG	N-CA-C	7.53	121.39	111.75
1	H	167	ARG	CD-NE-CZ	7.52	134.92	124.40
1	G	28	LYS	CA-C-O	-7.49	113.44	121.38
1	H	213	GLY	N-CA-C	7.49	123.61	114.69
1	D	167	ARG	CD-NE-CZ	7.49	134.88	124.40
1	E	238	TYR	CA-C-O	-7.46	110.94	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	167	ARG	CD-NE-CZ	7.42	134.78	124.40
1	G	9	THR	CA-C-N	7.38	135.97	121.58
1	G	9	THR	C-N-CA	7.38	135.97	121.58
1	B	261	ILE	N-CA-C	7.37	114.26	107.56
1	E	28	LYS	CA-C-O	-7.36	113.58	121.38
1	E	9	THR	CA-C-N	7.34	135.90	121.58
1	E	9	THR	C-N-CA	7.34	135.90	121.58
1	A	9	THR	CA-C-N	7.30	135.63	121.18
1	A	9	THR	C-N-CA	7.30	135.63	121.18
1	A	71	VAL	CB-CA-C	-7.25	99.66	110.82
1	B	72	ASN	CB-CA-C	-7.22	95.89	111.78
1	H	72	ASN	CA-CB-CG	-7.18	105.42	112.60
1	F	10	ASP	CA-CB-CG	7.17	119.77	112.60
1	B	71	VAL	CB-CA-C	-7.11	99.86	110.82
1	F	231	ARG	NE-CZ-NH2	7.09	125.58	119.20
1	E	71	VAL	CB-CA-C	-7.09	99.90	110.82
1	E	80	MET	CA-CB-CG	7.06	128.21	114.10
1	E	117	ASP	CA-CB-CG	-7.04	105.56	112.60
1	B	231	ARG	NE-CZ-NH2	6.99	125.49	119.20
1	B	195	ASN	N-CA-C	6.97	118.85	110.07
1	B	196	PRO	N-CA-C	6.95	118.02	110.58
1	E	72	ASN	CB-CA-C	-6.92	96.55	111.78
1	C	195	ASN	N-CA-C	6.92	118.78	110.07
1	G	72	ASN	CA-C-O	-6.90	113.81	121.89
1	D	297	SER	CA-CB-OG	6.90	124.89	111.10
1	H	296	ASN	CA-CB-CG	6.84	119.44	112.60
1	F	185	ASN	OD1-CG-ND2	-6.82	115.78	122.60
1	A	28	LYS	CA-C-N	-6.80	113.60	122.37
1	A	28	LYS	C-N-CA	-6.80	113.60	122.37
1	G	296	ASN	CA-CB-CG	6.77	119.37	112.60
1	D	213	GLY	N-CA-C	6.77	123.13	115.08
1	D	117	ASP	CA-CB-CG	-6.76	105.84	112.60
1	B	29	VAL	N-CA-CB	6.75	118.08	110.72
1	A	269	ASN	CA-C-O	6.74	127.56	120.42
1	C	130	ASN	CA-CB-CG	-6.69	105.91	112.60
1	C	213	GLY	N-CA-C	6.67	123.60	114.92
1	D	247	GLU	CA-C-N	6.64	127.31	119.94
1	D	247	GLU	C-N-CA	6.64	127.31	119.94
1	G	195	ASN	N-CA-C	6.63	118.42	110.07
1	B	28	LYS	CA-C-O	-6.62	114.36	121.38
1	C	28	LYS	CA-C-O	-6.61	114.38	121.38
1	D	28	LYS	CA-C-O	-6.59	114.40	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ASP	CA-CB-CG	-6.56	106.04	112.60
1	H	117	ASP	CA-CB-CG	-6.51	106.08	112.60
1	G	238	TYR	CA-C-O	-6.49	112.00	119.14
1	C	28	LYS	CA-C-N	-6.46	114.03	122.37
1	C	28	LYS	C-N-CA	-6.46	114.03	122.37
1	A	195	ASN	N-CA-C	6.45	118.20	110.07
1	C	147	THR	CA-C-N	6.45	132.44	120.95
1	C	147	THR	C-N-CA	6.45	132.44	120.95
1	A	28	LYS	CA-C-O	-6.44	114.55	121.38
1	F	28	LYS	CA-C-N	-6.43	114.07	122.37
1	F	28	LYS	C-N-CA	-6.43	114.07	122.37
1	F	71	VAL	CB-CA-C	-6.43	101.64	110.90
1	E	26	ASP	N-CA-CB	6.43	119.67	109.51
1	D	102	PRO	CA-C-N	6.39	131.12	120.64
1	D	102	PRO	C-N-CA	6.39	131.12	120.64
1	A	147	THR	CA-C-N	6.39	131.67	120.87
1	A	147	THR	C-N-CA	6.39	131.67	120.87
1	H	71	VAL	CB-CA-C	-6.38	101.72	110.90
1	F	40	LEU	N-CA-C	-6.34	105.56	113.55
1	H	177	PRO	CA-C-N	6.33	126.12	120.10
1	H	177	PRO	C-N-CA	6.33	126.12	120.10
1	C	80	MET	CA-CB-CG	6.28	126.65	114.10
1	D	231	ARG	NE-CZ-NH2	6.26	124.84	119.20
1	H	148	ASP	CB-CA-C	-6.25	96.86	109.68
1	D	296	ASN	CA-CB-CG	6.24	118.83	112.60
1	F	9	THR	CA-C-N	6.23	133.73	121.58
1	F	9	THR	C-N-CA	6.23	133.73	121.58
1	H	260	ASN	O-C-N	-6.23	115.46	122.93
1	H	105	VAL	N-CA-C	6.23	116.90	110.36
1	C	26	ASP	N-CA-CB	6.22	119.33	109.51
1	D	26	ASP	N-CA-CB	6.20	119.31	109.51
1	E	195	ASN	CA-C-N	6.20	124.12	119.66
1	E	195	ASN	C-N-CA	6.20	124.12	119.66
1	B	26	ASP	N-CA-CB	6.19	119.29	109.51
1	G	213	GLY	N-CA-C	6.17	122.43	115.08
1	G	29	VAL	N-CA-CB	6.17	117.45	110.72
1	H	79	ALA	N-CA-CB	-6.17	100.59	111.39
1	H	247	GLU	CA-C-N	6.17	126.96	119.99
1	H	247	GLU	C-N-CA	6.17	126.96	119.99
1	A	29	VAL	N-CA-CB	6.16	117.44	110.72
1	H	72	ASN	CA-C-O	-6.16	114.68	121.89
1	A	26	ASP	N-CA-CB	6.14	119.21	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	102	PRO	CA-C-N	6.14	130.83	120.64
1	F	102	PRO	C-N-CA	6.14	130.83	120.64
1	C	29	VAL	N-CA-CB	6.11	117.38	110.72
1	B	238	TYR	CA-C-O	-6.11	112.42	119.14
1	E	28	LYS	CA-C-N	-6.09	113.25	121.66
1	E	28	LYS	C-N-CA	-6.09	113.25	121.66
1	G	26	ASP	N-CA-CB	6.09	119.13	109.51
1	B	297	SER	CA-CB-OG	6.09	123.28	111.10
1	F	28	LYS	CA-C-O	-6.04	114.98	121.38
1	H	196	PRO	N-CA-C	6.03	118.06	110.70
1	E	269	ASN	CA-C-N	6.02	130.24	120.60
1	E	269	ASN	C-N-CA	6.02	130.24	120.60
1	H	147	THR	CA-C-N	6.02	131.92	120.97
1	H	147	THR	C-N-CA	6.02	131.92	120.97
1	G	261	ILE	CA-C-N	6.00	125.76	119.76
1	G	261	ILE	C-N-CA	6.00	125.76	119.76
1	E	29	VAL	N-CA-CB	5.98	117.05	110.53
1	A	148	ASP	CB-CA-C	-5.98	97.27	109.65
1	C	117	ASP	CA-CB-CG	-5.97	106.63	112.60
1	A	117	ASP	CA-CB-CG	-5.97	106.63	112.60
1	E	147	THR	CA-C-N	5.96	131.56	120.95
1	E	147	THR	C-N-CA	5.96	131.56	120.95
1	C	269	ASN	CA-C-O	5.95	126.72	120.42
1	B	231	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	F	234	TYR	CA-CB-CG	-5.93	103.22	113.90
1	D	195	ASN	N-CA-C	5.91	117.51	110.07
1	B	187	ARG	N-CA-C	5.90	118.50	111.71
1	F	296	ASN	CA-CB-CG	5.89	118.50	112.60
1	H	199	ASP	CA-CB-CG	5.89	118.49	112.60
1	B	147	THR	CA-C-N	5.89	131.43	120.95
1	B	147	THR	C-N-CA	5.89	131.43	120.95
1	E	114	VAL	N-CA-CB	5.86	116.45	111.64
1	F	80	MET	CA-CB-CG	5.86	125.82	114.10
1	C	217	LEU	CA-C-O	-5.86	115.37	120.88
1	F	26	ASP	N-CA-CB	5.85	118.76	109.51
1	A	175	ASN	CA-CB-CG	-5.85	106.75	112.60
1	D	196	PRO	N-CA-C	5.85	117.83	110.70
1	F	269	ASN	CA-C-N	5.84	129.95	120.60
1	F	269	ASN	C-N-CA	5.84	129.95	120.60
1	D	177	PRO	CA-C-N	5.84	127.13	120.53
1	D	177	PRO	C-N-CA	5.84	127.13	120.53
1	A	269	ASN	CA-C-N	5.84	129.94	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ASN	C-N-CA	5.84	129.94	120.60
1	H	234	TYR	CA-CB-CG	-5.83	103.40	113.90
1	E	80	MET	CB-CA-C	-5.82	100.14	109.75
1	E	48	ILE	N-CA-CB	5.82	117.06	110.72
1	H	102	PRO	CA-C-N	5.82	130.30	120.64
1	H	102	PRO	C-N-CA	5.82	130.30	120.64
1	E	196	PRO	N-CA-C	5.82	116.80	110.58
1	A	102	PRO	CA-C-N	5.81	130.43	121.19
1	A	102	PRO	C-N-CA	5.81	130.43	121.19
1	D	147	THR	CA-C-N	5.79	131.25	120.95
1	D	147	THR	C-N-CA	5.79	131.25	120.95
1	A	80	MET	CA-CB-CG	5.78	125.67	114.10
1	G	196	PRO	N-CA-C	5.78	117.75	110.70
1	B	175	ASN	CA-CB-CG	-5.78	106.82	112.60
1	G	17	ARG	CA-C-O	5.78	127.57	121.33
1	F	148	ASP	CB-CA-C	-5.77	97.61	110.19
1	A	196	PRO	N-CA-C	5.77	117.74	110.70
1	C	296	ASN	CA-CB-CG	5.77	118.37	112.60
1	D	183	GLN	CA-C-O	-5.76	114.44	120.55
1	G	48	ILE	N-CA-CB	5.76	117.00	110.72
1	G	80	MET	CA-CB-CG	5.74	125.58	114.10
1	B	80	MET	CB-CA-C	-5.72	100.67	110.22
1	E	10	ASP	CA-CB-CG	5.71	118.31	112.60
1	D	234	TYR	CA-CB-CG	-5.71	103.63	113.90
1	D	269	ASN	CA-C-N	5.71	129.73	120.60
1	D	269	ASN	C-N-CA	5.71	129.73	120.60
1	D	130	ASN	CA-CB-CG	-5.70	106.90	112.60
1	D	29	VAL	N-CA-CB	5.70	116.93	110.72
1	E	214	ALA	N-CA-C	5.70	119.33	112.38
1	B	80	MET	CA-CB-CG	5.70	125.49	114.10
1	C	17	ARG	CA-C-O	5.70	127.37	120.99
1	C	148	ASP	CB-CA-C	-5.70	96.92	110.02
1	G	80	MET	CB-CA-C	-5.68	100.37	109.75
1	A	238	TYR	CA-C-O	-5.68	112.89	119.14
1	F	26	ASP	CA-CB-CG	5.66	118.26	112.60
1	C	10	ASP	CA-CB-CG	5.65	118.25	112.60
1	C	72	ASN	CA-C-O	-5.65	115.28	121.89
1	C	48	ILE	N-CA-CB	5.64	116.87	110.72
1	B	48	ILE	N-CA-CB	5.63	116.86	110.72
1	H	9	THR	CA-C-N	5.62	132.54	121.58
1	H	9	THR	C-N-CA	5.62	132.54	121.58
1	F	29	VAL	N-CA-CB	5.62	116.85	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ASP	CA-CB-CG	5.62	118.22	112.60
1	H	237	LYS	O-C-N	5.61	128.07	122.12
1	G	234	TYR	CA-CB-CG	-5.61	103.81	113.90
1	H	26	ASP	CA-CB-CG	5.60	118.20	112.60
1	F	195	ASN	OD1-CG-ND2	5.60	128.20	122.60
1	D	189	TYR	O-C-N	-5.59	115.38	122.26
1	E	175	ASN	CA-CB-CG	-5.59	107.01	112.60
1	C	175	ASN	CA-CB-CG	-5.58	107.02	112.60
1	D	308	ASN	CA-CB-CG	5.54	118.14	112.60
1	A	10	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	231	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	F	196	PRO	N-CA-C	5.52	117.44	110.70
1	G	72	ASN	CA-CB-CG	-5.52	107.08	112.60
1	A	297	SER	CA-CB-OG	5.51	122.12	111.10
1	D	269	ASN	OD1-CG-ND2	5.51	128.11	122.60
1	C	247	GLU	CA-C-N	5.51	126.05	119.94
1	C	247	GLU	C-N-CA	5.51	126.05	119.94
1	E	73	GLU	N-CA-C	-5.51	106.56	113.28
1	D	80	MET	CA-CB-CG	5.50	125.10	114.10
1	D	166	HIS	CA-CB-CG	-5.50	108.30	113.80
1	G	187	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	G	10	ASP	N-CA-CB	-5.47	101.23	110.41
1	B	269	ASN	OD1-CG-ND2	5.46	128.06	122.60
1	B	199	ASP	CA-CB-CG	5.45	118.05	112.60
1	E	40	LEU	N-CA-C	-5.44	106.70	113.55
1	B	230	LEU	CA-C-O	5.44	126.53	120.82
1	F	147	THR	CA-C-N	5.43	131.27	121.06
1	F	147	THR	C-N-CA	5.43	131.27	121.06
1	E	187	ARG	N-CA-C	5.42	117.94	111.71
1	G	269	ASN	CA-C-N	5.42	129.27	120.60
1	G	269	ASN	C-N-CA	5.42	129.27	120.60
1	A	199	ASP	CA-CB-CG	5.42	118.02	112.60
1	F	175	ASN	OD1-CG-ND2	5.41	128.01	122.60
1	A	72	ASN	OD1-CG-ND2	5.40	128.00	122.60
1	H	26	ASP	N-CA-CB	5.40	118.04	109.51
1	D	48	ILE	N-CA-CB	5.40	116.60	110.72
1	G	28	LYS	CA-C-N	-5.39	115.41	122.37
1	G	28	LYS	C-N-CA	-5.39	115.41	122.37
1	B	18	THR	CA-C-O	-5.39	115.07	121.16
1	B	148	ASP	CB-CA-C	-5.36	97.68	110.02
1	G	237	LYS	O-C-N	5.36	127.59	122.07
1	D	329	ASN	CA-CB-CG	5.36	117.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	G	9	THR	CA-C-O	5.35	125.55	119.18
1	F	70	GLY	N-CA-C	5.34	117.31	110.96
1	E	130	ASN	CA-CB-CG	-5.33	107.27	112.60
1	E	240	GLU	N-CA-C	5.33	117.17	110.24
1	C	26	ASP	CA-CB-CG	5.32	117.92	112.60
1	H	48	ILE	N-CA-CB	5.31	116.51	110.72
1	F	73	GLU	N-CA-C	-5.30	106.81	113.28
1	A	166	HIS	CA-CB-CG	-5.30	108.50	113.80
1	A	200	ILE	O-C-N	-5.30	117.36	122.92
1	A	130	ASN	CA-CB-CG	-5.29	107.31	112.60
1	D	72	ASN	OD1-CG-ND2	5.29	127.89	122.60
1	D	157	GLU	CG-CD-OE1	5.29	130.57	118.40
1	G	308	ASN	CA-CB-CG	5.28	117.88	112.60
1	F	1	CYS	CA-CB-SG	5.28	126.54	114.40
1	B	73	GLU	N-CA-C	-5.27	106.69	113.23
1	B	157	GLU	CG-CD-OE1	5.27	130.53	118.40
1	A	163	ILE	CA-C-O	-5.27	114.50	120.98
1	C	234	TYR	CA-CB-CG	-5.26	104.43	113.90
1	B	102	PRO	CA-C-N	5.26	129.26	120.64
1	B	102	PRO	C-N-CA	5.26	129.26	120.64
1	C	298	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	C	231	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	D	80	MET	CB-CA-C	-5.25	101.09	109.75
1	E	71	VAL	CA-C-N	5.24	131.93	122.02
1	E	71	VAL	C-N-CA	5.24	131.93	122.02
1	A	157	GLU	CG-CD-OE1	5.24	130.44	118.40
1	F	244	ASN	CA-C-O	-5.23	115.75	121.14
1	D	10	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	296	ASN	CA-CB-CG	5.22	117.82	112.60
1	B	130	ASN	CA-CB-CG	-5.21	107.39	112.60
1	D	214	ALA	N-CA-C	5.21	119.12	112.87
1	H	29	VAL	N-CA-CB	5.20	116.20	110.53
1	B	296	ASN	CA-CB-CG	5.20	117.80	112.60
1	F	247	GLU	CA-C-O	5.20	126.06	120.55
1	D	72	ASN	CA-CB-CG	-5.20	107.40	112.60
1	B	308	ASN	CA-CB-CG	5.19	117.79	112.60
1	C	329	ASN	CA-CB-CG	5.19	117.79	112.60
1	G	187	ARG	N-CA-C	5.18	118.39	111.75
1	A	118	ASP	CA-C-N	5.18	127.09	120.56
1	A	118	ASP	C-N-CA	5.18	127.09	120.56
1	G	113	CYS	CA-C-N	-5.17	117.86	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	113	CYS	C-N-CA	-5.17	117.86	123.08
1	D	331	VAL	CA-C-O	-5.15	116.41	122.13
1	A	234	TYR	CA-CB-CG	-5.15	104.63	113.90
1	C	187	ARG	N-CA-C	5.15	117.63	111.71
1	G	40	LEU	N-CA-C	-5.15	107.06	113.55
1	H	301	ALA	CA-C-O	5.15	126.26	120.70
1	C	29	VAL	CB-CA-C	5.15	117.29	110.91
1	G	147	THR	CA-C-N	5.15	130.11	120.95
1	G	147	THR	C-N-CA	5.15	130.11	120.95
1	G	102	PRO	CA-C-N	5.14	129.58	121.09
1	G	102	PRO	C-N-CA	5.14	129.58	121.09
1	G	298	ARG	NH1-CZ-NH2	5.14	125.99	119.30
1	B	185	ASN	O-C-N	-5.13	116.68	122.12
1	D	148	ASP	CB-CA-C	-5.13	98.22	110.02
1	E	195	ASN	N-CA-C	5.12	116.52	110.07
1	E	114	VAL	N-CA-C	-5.12	107.58	111.62
1	E	308	ASN	CA-CB-CG	5.11	117.71	112.60
1	F	71	VAL	N-CA-CB	5.11	121.06	112.47
1	C	105	VAL	N-CA-C	5.10	115.32	110.42
1	C	177	PRO	CA-C-N	5.10	126.00	120.44
1	C	177	PRO	C-N-CA	5.10	126.00	120.44
1	C	196	PRO	N-CA-C	5.10	116.92	110.70
1	H	72	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	B	28	LYS	CA-C-N	-5.08	115.81	122.37
1	B	28	LYS	C-N-CA	-5.08	115.81	122.37
1	F	229	PHE	CA-C-N	5.07	127.39	120.54
1	F	229	PHE	C-N-CA	5.07	127.39	120.54
1	D	105	VAL	N-CA-C	5.07	115.79	110.62
1	F	48	ILE	N-CA-CB	5.07	116.24	110.72
1	B	292	LYS	N-CA-CB	5.07	120.36	111.55
1	H	269	ASN	CA-C-N	5.07	129.18	120.72
1	H	269	ASN	C-N-CA	5.07	129.18	120.72
1	D	329	ASN	CA-C-O	-5.06	115.35	121.32
1	E	26	ASP	CA-CB-CG	5.05	117.65	112.60
1	E	329	ASN	CA-CB-CG	5.05	117.65	112.60
1	E	72	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	F	67	LEU	CA-C-O	5.04	126.06	120.71
1	A	26	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	175	ASN	N-CA-C	5.04	116.39	109.29
1	C	118	ASP	CA-C-N	5.03	126.89	120.56
1	C	118	ASP	C-N-CA	5.03	126.89	120.56
1	H	18	THR	CA-C-O	-5.03	115.48	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	292	LYS	N-CA-CB	5.02	120.51	111.37
1	C	166	HIS	CA-CB-CG	-5.02	108.78	113.80
1	H	239	THR	N-CA-CB	5.01	117.39	110.17
1	A	7	ARG	CA-C-O	-5.01	114.95	120.36
1	C	292	LYS	N-CA-CB	5.00	120.47	111.37
1	G	181	TRP	CA-C-N	5.00	126.94	120.44
1	G	181	TRP	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ASP	Mainchain
1	A	72	ASN	Mainchain
1	B	148	ASP	Mainchain
1	B	96	GLY	Mainchain
1	C	148	ASP	Mainchain
1	C	72	ASN	Mainchain
1	E	148	ASP	Mainchain
1	E	72	ASN	Mainchain
1	E	96	GLY	Mainchain
1	G	72	ASN	Mainchain
1	H	72	ASN	Mainchain

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	2605	0	2582	91	0
1	B	2605	0	2582	92	0
1	C	2605	0	2582	96	0
1	D	2605	0	2582	83	0
1	E	2605	0	2582	100	0
1	F	2605	0	2582	107	0
1	G	2605	0	2582	93	0
1	H	2605	0	2582	113	0
2	A	346	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	348	0	0	10	0
2	C	350	0	0	10	0
2	D	356	0	0	12	0
2	E	353	0	0	12	0
2	F	350	0	0	15	0
2	G	351	0	0	15	0
2	H	346	0	0	17	0
All	All	23640	0	20656	701	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 17.

All (701) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:THR:HG21	1:C:187:ARG:HH22	1.17	1.08
1:E:187:ARG:HH22	1:G:85:THR:HG21	1.15	1.04
1:E:85:THR:HG21	1:G:187:ARG:HH22	1.19	1.03
1:B:187:ARG:HH22	1:D:85:THR:HG21	1.24	1.00
1:A:187:ARG:HH22	1:C:85:THR:HG21	1.23	1.00
1:B:85:THR:HG21	1:D:187:ARG:HH22	1.23	1.00
1:F:187:ARG:HH22	1:H:85:THR:HG21	1.29	0.98
1:F:85:THR:HG21	1:H:187:ARG:HH22	1.29	0.98
1:H:71:VAL:HG22	1:H:282:MET:HG2	1.53	0.89
1:C:235:TRP:O	1:C:239:THR:HG23	1.78	0.84
1:D:235:TRP:O	1:D:239:THR:HG23	1.78	0.83
1:H:95:LYS:H	1:H:95:LYS:HD2	1.44	0.83
1:B:71:VAL:HG22	1:B:282:MET:HG2	1.61	0.82
1:F:95:LYS:H	1:F:95:LYS:HD2	1.44	0.82
1:B:95:LYS:H	1:B:95:LYS:HD2	1.43	0.81
1:D:95:LYS:H	1:D:95:LYS:HD2	1.46	0.81
1:A:71:VAL:HG22	1:A:282:MET:HG2	1.63	0.80
1:A:235:TRP:O	1:A:239:THR:HG23	1.82	0.80
1:D:71:VAL:HG22	1:D:282:MET:HG2	1.64	0.79
1:E:235:TRP:O	1:E:239:THR:HG23	1.81	0.79
1:G:235:TRP:O	1:G:239:THR:HG23	1.82	0.79
1:G:71:VAL:HG22	1:G:282:MET:HG2	1.63	0.79
1:C:40:LEU:HD21	1:C:126:TYR:HE1	1.46	0.78
1:B:71:VAL:HG13	1:B:77:MET:HG2	1.65	0.78
1:G:95:LYS:H	1:G:95:LYS:HD2	1.47	0.78
1:A:95:LYS:H	1:A:95:LYS:HD2	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:VAL:HG13	1:D:77:MET:HG2	1.66	0.78
1:E:95:LYS:HD2	1:E:95:LYS:H	1.49	0.77
1:F:54:PHE:HE1	1:F:67:LEU:HD13	1.47	0.77
1:H:235:TRP:O	1:H:239:THR:HG23	1.84	0.77
1:E:71:VAL:HG22	1:E:282:MET:HG2	1.65	0.76
1:C:95:LYS:H	1:C:95:LYS:HD2	1.48	0.76
1:B:84:ALA:O	1:B:85:THR:HB	1.86	0.75
1:C:84:ALA:O	1:C:85:THR:HB	1.85	0.75
1:C:71:VAL:HG22	1:C:282:MET:HG2	1.68	0.74
1:E:54:PHE:HE1	1:E:67:LEU:HD13	1.52	0.73
1:H:40:LEU:HD21	1:H:126:TYR:HE1	1.53	0.73
1:B:235:TRP:O	1:B:239:THR:HG23	1.89	0.73
1:D:84:ALA:O	1:D:85:THR:HB	1.88	0.73
1:F:71:VAL:HG22	1:F:282:MET:HG2	1.70	0.73
1:H:155:VAL:HG13	1:H:173:MET:HE3	1.70	0.73
1:D:54:PHE:HE1	1:D:67:LEU:HD13	1.54	0.72
1:E:40:LEU:HD21	1:E:126:TYR:HE1	1.54	0.72
1:B:54:PHE:HE1	1:B:67:LEU:HD13	1.55	0.72
1:A:84:ALA:O	1:A:85:THR:HB	1.90	0.72
1:B:89:TYR:HB2	1:B:130:ASN:HD22	1.54	0.71
1:E:84:ALA:O	1:E:85:THR:HB	1.89	0.71
1:C:71:VAL:HG13	1:C:77:MET:HG2	1.71	0.71
1:A:89:TYR:HB2	1:A:130:ASN:HD22	1.54	0.71
1:G:40:LEU:HD21	1:G:126:TYR:HE1	1.55	0.71
1:C:54:PHE:HE1	1:C:67:LEU:HD13	1.56	0.71
1:E:155:VAL:HG13	1:E:173:MET:CE	2.21	0.71
1:D:40:LEU:HD21	1:D:126:TYR:HE1	1.55	0.70
1:H:84:ALA:O	1:H:85:THR:HB	1.90	0.70
1:H:71:VAL:HG13	1:H:77:MET:HG2	1.73	0.70
1:H:89:TYR:HB2	1:H:130:ASN:HD22	1.56	0.69
1:D:89:TYR:HB2	1:D:130:ASN:HD22	1.56	0.69
1:A:327:GLN:HB3	1:A:331:VAL:HG23	1.75	0.69
1:F:89:TYR:HB2	1:F:130:ASN:HD22	1.58	0.69
1:A:54:PHE:HE1	1:A:67:LEU:HD13	1.57	0.68
1:G:84:ALA:O	1:G:85:THR:HB	1.93	0.68
1:B:40:LEU:HD21	1:B:126:TYR:HE1	1.58	0.68
1:E:89:TYR:HB2	1:E:130:ASN:HD22	1.58	0.68
1:D:155:VAL:HG13	1:D:173:MET:CE	2.23	0.68
1:F:219:LEU:HD23	1:F:220:PRO:HD2	1.76	0.68
1:B:155:VAL:HG13	1:B:173:MET:CE	2.25	0.67
1:C:89:TYR:HB2	1:C:130:ASN:HD22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:TRP:O	1:F:239:THR:HG23	1.95	0.67
1:A:40:LEU:HD21	1:A:126:TYR:HE1	1.60	0.66
1:F:40:LEU:HD21	1:F:126:TYR:HE1	1.59	0.66
1:A:155:VAL:HG22	1:A:173:MET:HE3	1.78	0.66
1:G:54:PHE:HE2	1:G:67:LEU:HD13	1.61	0.66
1:A:71:VAL:HG13	1:A:77:MET:HG2	1.76	0.66
1:E:72:ASN:HB3	1:E:74:LYS:H	1.61	0.65
1:E:71:VAL:HG13	1:E:77:MET:HG2	1.77	0.65
1:H:72:ASN:HB3	1:H:74:LYS:H	1.61	0.65
1:A:85:THR:HG21	1:C:187:ARG:NH2	2.02	0.65
1:E:209:PRO:HG2	2:E:2665:HOH:O	1.96	0.65
1:C:155:VAL:HG13	1:C:173:MET:CE	2.27	0.64
1:F:85:THR:HG21	1:H:187:ARG:NH2	2.08	0.64
1:F:1:CYS:HB3	1:F:18:THR:O	1.97	0.64
1:F:243:LYS:HE3	2:F:1949:HOH:O	1.98	0.64
1:E:298:ARG:HG3	1:H:298:ARG:HG3	1.79	0.64
1:H:31:ILE:HD12	1:H:307:GLU:HG3	1.79	0.64
1:A:74:LYS:HG3	1:A:114:VAL:HG22	1.79	0.64
1:B:72:ASN:HB3	1:B:74:LYS:H	1.63	0.64
1:E:219:LEU:HD23	1:E:220:PRO:HD2	1.78	0.64
1:C:155:VAL:HG13	1:C:173:MET:HE3	1.80	0.63
1:E:187:ARG:NH2	1:G:85:THR:HG21	2.00	0.63
1:E:323:GLN:HE21	1:H:250:THR:CG2	2.10	0.63
1:F:71:VAL:HG13	1:F:77:MET:HG2	1.80	0.63
1:H:327:GLN:HB3	1:H:331:VAL:HG23	1.79	0.63
1:A:187:ARG:NH2	1:C:85:THR:HG21	2.05	0.63
1:D:12:LYS:HD3	1:D:245:GLU:HB2	1.80	0.63
1:F:187:ARG:NH2	1:H:85:THR:HG21	2.08	0.63
1:G:89:TYR:HB2	1:G:130:ASN:HD22	1.62	0.63
1:F:7:ARG:HB2	2:F:1976:HOH:O	1.98	0.63
1:G:72:ASN:HB3	1:G:74:LYS:H	1.64	0.63
1:C:327:GLN:HB3	1:C:331:VAL:HG23	1.81	0.62
1:A:250:THR:CG2	1:D:323:GLN:HE21	2.12	0.62
1:B:74:LYS:HG3	1:B:114:VAL:HG22	1.82	0.62
1:E:334:MET:O	1:H:245:GLU:HB3	1.99	0.62
1:F:115:THR:HA	1:F:148:ASP:OD1	1.98	0.62
1:G:7:ARG:HB2	2:G:2326:HOH:O	2.00	0.62
1:E:155:VAL:HG13	1:E:173:MET:HE3	1.81	0.62
1:B:7:ARG:HB2	2:B:535:HOH:O	1.99	0.62
1:B:155:VAL:HG13	1:B:173:MET:HE3	1.81	0.62
1:C:243:LYS:HE3	2:C:555:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:ALA:O	1:F:85:THR:HB	2.00	0.62
1:A:74:LYS:CG	1:A:114:VAL:HG22	2.30	0.61
1:B:323:GLN:HE21	1:C:250:THR:CG2	2.13	0.61
1:C:72:ASN:HB3	1:C:74:LYS:H	1.65	0.61
1:A:31:ILE:HD12	1:A:307:GLU:HG3	1.80	0.61
1:A:72:ASN:HB3	1:A:74:LYS:H	1.65	0.61
1:B:327:GLN:HB3	1:B:331:VAL:HG23	1.81	0.61
1:E:327:GLN:HB3	1:E:331:VAL:HG23	1.82	0.61
1:C:7:ARG:HB2	2:C:577:HOH:O	2.00	0.61
1:G:71:VAL:HG13	1:G:77:MET:HG2	1.83	0.61
1:F:12:LYS:HD3	1:F:245:GLU:HB2	1.82	0.61
1:G:209:PRO:HG2	2:G:1965:HOH:O	2.01	0.61
1:H:219:LEU:HD23	1:H:220:PRO:HD2	1.82	0.60
1:E:155:VAL:HG22	1:E:173:MET:HE3	1.81	0.60
1:F:327:GLN:HB3	1:F:331:VAL:HG23	1.82	0.60
1:F:328:LEU:HG	2:G:2408:HOH:O	2.01	0.60
1:G:219:LEU:HD23	1:G:220:PRO:HD2	1.83	0.60
1:A:298:ARG:HG3	1:D:298:ARG:HG3	1.83	0.60
1:G:155:VAL:HG22	1:G:173:MET:HE3	1.84	0.60
1:C:74:LYS:CG	1:C:114:VAL:HG22	2.32	0.60
1:E:250:THR:CG2	1:H:323:GLN:HE21	2.15	0.60
1:D:327:GLN:HB3	1:D:331:VAL:HG23	1.84	0.60
1:F:167:ARG:HD2	2:F:1984:HOH:O	2.01	0.60
1:E:7:ARG:HB2	2:E:1626:HOH:O	2.01	0.59
1:B:250:THR:CG2	1:C:323:GLN:HE21	2.15	0.59
2:B:598:HOH:O	1:C:328:LEU:HG	2.02	0.59
1:B:74:LYS:CG	1:B:114:VAL:HG22	2.33	0.59
1:A:219:LEU:HD23	1:A:220:PRO:HD2	1.85	0.59
1:B:250:THR:HG21	1:C:323:GLN:HE21	1.67	0.59
1:C:31:ILE:HD12	1:C:307:GLU:HG3	1.84	0.59
1:G:327:GLN:HB3	1:G:331:VAL:HG23	1.84	0.59
1:H:61:ASP:HB3	1:H:135:ILE:HD11	1.84	0.59
1:A:155:VAL:HG13	1:A:173:MET:CE	2.32	0.59
1:D:155:VAL:HG13	1:D:173:MET:HE3	1.84	0.59
1:E:85:THR:HG21	1:G:187:ARG:NH2	2.04	0.59
1:F:333:VAL:HA	2:G:2200:HOH:O	2.03	0.59
1:G:61:ASP:HB3	1:G:135:ILE:HD11	1.85	0.59
1:B:1:CYS:HB3	1:B:18:THR:O	2.02	0.59
1:F:265:VAL:CG1	1:G:239:THR:HG22	2.33	0.58
1:B:323:GLN:HE21	1:C:250:THR:HG21	1.68	0.58
1:H:9:THR:OG1	1:H:243:LYS:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:CYS:HB3	1:A:18:THR:O	2.02	0.58
1:A:12:LYS:HD3	1:A:245:GLU:HB2	1.84	0.58
1:C:74:LYS:HG3	1:C:114:VAL:HG22	1.84	0.58
1:G:155:VAL:HG13	1:G:173:MET:CE	2.33	0.58
1:H:1:CYS:HB3	1:H:18:THR:O	2.04	0.58
1:H:74:LYS:HG3	1:H:114:VAL:HG22	1.84	0.58
1:B:12:LYS:HD3	1:B:245:GLU:HB2	1.84	0.58
1:E:243:LYS:HE3	2:E:1599:HOH:O	2.03	0.58
1:F:9:THR:OG1	1:F:243:LYS:HA	2.04	0.58
1:E:74:LYS:HG3	1:E:114:VAL:HG22	1.85	0.58
1:A:250:THR:HG21	1:D:323:GLN:HE21	1.69	0.58
1:F:209:PRO:HG2	2:G:2315:HOH:O	2.04	0.58
1:B:209:PRO:HG2	2:C:570:HOH:O	2.04	0.57
1:H:243:LYS:HE3	2:H:576:HOH:O	2.03	0.57
1:D:95:LYS:H	1:D:95:LYS:CD	2.15	0.57
1:E:74:LYS:CG	1:E:114:VAL:HG22	2.35	0.57
1:E:265:VAL:CG1	1:H:239:THR:HG22	2.34	0.57
1:B:31:ILE:HD12	1:B:307:GLU:HG3	1.86	0.57
1:B:95:LYS:H	1:B:95:LYS:CD	2.14	0.57
1:H:54:PHE:HE1	1:H:67:LEU:HD13	1.68	0.57
1:A:323:GLN:HE21	1:D:250:THR:CG2	2.18	0.57
1:D:31:ILE:HD12	1:D:307:GLU:HG3	1.87	0.57
1:F:74:LYS:CG	1:F:114:VAL:HG22	2.34	0.57
1:B:85:THR:HG21	1:D:187:ARG:NH2	2.07	0.57
1:A:7:ARG:HB2	2:A:513:HOH:O	2.04	0.57
1:D:61:ASP:HB3	1:D:135:ILE:HD11	1.86	0.57
1:E:83:TYR:CE2	1:E:157:GLU:HG2	2.40	0.57
1:B:239:THR:HG22	1:C:265:VAL:CG1	2.35	0.56
1:C:219:LEU:HD23	1:C:220:PRO:HD2	1.87	0.56
1:D:74:LYS:CG	1:D:114:VAL:HG22	2.35	0.56
2:B:527:HOH:O	1:C:209:PRO:HG2	2.05	0.56
1:C:167:ARG:HD2	2:C:584:HOH:O	2.04	0.56
1:G:31:ILE:HD12	1:G:307:GLU:HG3	1.86	0.56
1:A:265:VAL:CG1	1:D:239:THR:HG22	2.35	0.56
1:E:95:LYS:H	1:E:95:LYS:CD	2.18	0.56
1:E:12:LYS:HD3	1:E:245:GLU:HB2	1.86	0.56
1:F:175:ASN:HB2	1:F:225:PRO:HB3	1.88	0.56
2:B:443:HOH:O	1:C:250:THR:HG21	2.05	0.56
1:A:250:THR:HG21	2:D:508:HOH:O	2.05	0.56
1:F:72:ASN:HB3	1:F:74:LYS:H	1.71	0.56
1:G:74:LYS:HG3	1:G:114:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:THR:OG1	1:G:243:LYS:HA	2.05	0.56
1:A:209:PRO:HG2	2:D:596:HOH:O	2.05	0.55
1:A:333:VAL:HA	2:D:502:HOH:O	2.06	0.55
1:A:95:LYS:H	1:A:95:LYS:CD	2.19	0.55
1:C:155:VAL:HG22	1:C:173:MET:HE3	1.88	0.55
1:D:243:LYS:HE3	2:D:582:HOH:O	2.05	0.55
1:C:40:LEU:HD21	1:C:126:TYR:CE1	2.34	0.55
1:F:83:TYR:CZ	1:F:157:GLU:HG2	2.41	0.55
1:H:6:ILE:HD12	1:H:252:LEU:HG	1.89	0.55
1:F:219:LEU:CD2	1:F:220:PRO:HD2	2.36	0.55
1:H:115:THR:HA	1:H:148:ASP:OD1	2.07	0.55
1:E:239:THR:HG22	1:H:265:VAL:CG1	2.37	0.55
1:D:263:LYS:HD2	1:D:294:TYR:CE2	2.42	0.55
1:F:6:ILE:HB	2:F:1809:HOH:O	2.07	0.55
1:F:333:VAL:HG11	2:F:1967:HOH:O	2.07	0.55
1:C:167:ARG:HH11	1:C:167:ARG:HG2	1.72	0.54
1:C:193:THR:HB	1:C:194:PRO:CD	2.36	0.54
1:E:222:ASP:OD1	1:E:224:THR:HG23	2.08	0.54
1:F:155:VAL:HG13	1:F:173:MET:CE	2.37	0.54
1:A:245:GLU:HB3	1:D:334:MET:O	2.08	0.54
1:C:1:CYS:HB3	1:C:18:THR:O	2.06	0.54
1:E:250:THR:HG21	1:H:323:GLN:HE21	1.71	0.54
1:G:190:ILE:HD12	1:H:198:GLN:O	2.08	0.54
1:H:12:LYS:HD3	1:H:245:GLU:HB2	1.89	0.54
1:E:6:ILE:HB	2:E:1459:HOH:O	2.07	0.54
1:G:246:THR:O	1:G:250:THR:HG23	2.08	0.54
1:C:95:LYS:H	1:C:95:LYS:CD	2.18	0.54
1:F:61:ASP:HB3	1:F:135:ILE:HD11	1.90	0.54
1:D:155:VAL:HG22	1:D:173:MET:HE3	1.89	0.54
1:E:83:TYR:CZ	1:E:157:GLU:HG2	2.42	0.54
1:H:169:THR:HB	1:H:179:TYR:CZ	2.43	0.54
1:B:61:ASP:HB3	1:B:135:ILE:HD11	1.90	0.54
1:B:187:ARG:NH2	1:D:85:THR:HG21	2.09	0.54
1:H:167:ARG:HH11	1:H:167:ARG:HG2	1.70	0.54
1:C:24:GLU:OE1	1:C:321:ARG:NH1	2.41	0.54
2:A:413:HOH:O	1:D:333:VAL:HA	2.08	0.54
1:D:167:ARG:HG2	1:D:167:ARG:HH11	1.73	0.54
1:D:219:LEU:HD23	1:D:220:PRO:HD2	1.88	0.54
1:E:323:GLN:HG3	1:E:325:ILE:CD1	2.37	0.54
1:F:167:ARG:HG2	1:F:167:ARG:HH11	1.72	0.54
2:A:419:HOH:O	1:D:250:THR:HG21	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1850:HOH:O	1:G:333:VAL:HA	2.08	0.54
2:F:1862:HOH:O	1:G:250:THR:HG21	2.07	0.53
1:D:1:CYS:HB3	1:D:18:THR:O	2.08	0.53
1:E:115:THR:HA	1:E:148:ASP:OD1	2.08	0.53
1:F:72:ASN:ND2	1:F:110:LEU:O	2.30	0.53
1:H:155:VAL:HG13	1:H:173:MET:CE	2.37	0.53
1:D:127:THR:HG22	1:D:129:LEU:HD23	1.91	0.53
1:G:224:THR:O	1:G:228:ARG:HG3	2.09	0.53
1:H:6:ILE:HB	2:H:472:HOH:O	2.08	0.53
1:C:323:GLN:HG3	1:C:325:ILE:CD1	2.39	0.53
1:E:1:CYS:HB3	1:E:18:THR:O	2.08	0.53
1:F:74:LYS:HG3	1:F:114:VAL:HG22	1.90	0.53
1:A:323:GLN:HG3	1:A:325:ILE:CD1	2.39	0.53
1:E:31:ILE:HD12	1:E:307:GLU:HG3	1.89	0.53
1:E:323:GLN:HG3	1:E:325:ILE:HD11	1.89	0.53
1:B:9:THR:OG1	1:B:243:LYS:HA	2.08	0.53
1:C:12:LYS:HD3	1:C:245:GLU:HB2	1.91	0.53
1:C:323:GLN:HG3	1:C:325:ILE:HD11	1.90	0.53
1:E:250:THR:HG21	2:H:506:HOH:O	2.09	0.53
1:E:61:ASP:HB3	1:E:135:ILE:HD11	1.90	0.53
1:E:176:SER:HB3	1:E:177:PRO:HA	1.91	0.53
1:H:323:GLN:HG3	1:H:325:ILE:CD1	2.39	0.53
1:F:193:THR:HB	1:F:194:PRO:CD	2.39	0.53
1:A:239:THR:HG22	1:D:265:VAL:CG1	2.39	0.52
1:F:331:VAL:HG21	1:G:301:ALA:HB3	1.91	0.52
1:B:219:LEU:HD23	1:B:220:PRO:HD2	1.90	0.52
1:H:67:LEU:O	1:H:80:MET:HE2	2.09	0.52
1:B:323:GLN:HG3	1:B:325:ILE:CD1	2.38	0.52
1:B:167:ARG:HG2	1:B:167:ARG:HH11	1.74	0.52
1:C:83:TYR:CZ	1:C:157:GLU:HG2	2.44	0.52
1:F:95:LYS:H	1:F:95:LYS:CD	2.16	0.52
1:H:7:ARG:HB2	2:H:596:HOH:O	2.09	0.52
1:A:61:ASP:HB3	1:A:135:ILE:HD11	1.90	0.52
1:A:327:GLN:OE1	1:A:331:VAL:HB	2.09	0.52
1:B:243:LYS:HE3	2:B:513:HOH:O	2.08	0.52
1:D:74:LYS:HG3	1:D:114:VAL:HG22	1.90	0.52
1:C:9:THR:OG1	1:C:243:LYS:HA	2.10	0.52
1:H:241:LYS:HG2	2:H:561:HOH:O	2.09	0.52
1:A:9:THR:OG1	1:A:243:LYS:HA	2.10	0.52
1:A:85:THR:HG22	1:A:86:PHE:CD2	2.45	0.52
1:A:328:LEU:HG	2:D:666:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:LYS:H	1:H:95:LYS:CD	2.17	0.52
1:D:72:ASN:HB3	1:D:74:LYS:H	1.74	0.52
1:H:327:GLN:OE1	1:H:331:VAL:HB	2.09	0.52
1:A:6:ILE:HB	2:A:387:HOH:O	2.09	0.51
1:E:219:LEU:CD2	1:E:220:PRO:HD2	2.38	0.51
1:E:333:VAL:HA	2:H:500:HOH:O	2.08	0.51
1:G:74:LYS:CG	1:G:114:VAL:HG22	2.40	0.51
1:C:246:THR:O	1:C:250:THR:HG23	2.10	0.51
1:F:250:THR:HG21	1:G:323:GLN:HE21	1.75	0.51
1:B:7:ARG:HD3	2:B:535:HOH:O	2.10	0.51
1:B:239:THR:HG22	1:C:262:PRO:HB2	1.90	0.51
1:E:127:THR:HG22	1:E:129:LEU:HD23	1.92	0.51
1:H:83:TYR:CE2	1:H:157:GLU:HG2	2.44	0.51
1:D:83:TYR:CZ	1:D:157:GLU:HG2	2.46	0.51
1:F:83:TYR:CE2	1:F:157:GLU:HG2	2.46	0.51
1:A:263:LYS:HD2	1:A:294:TYR:CE2	2.46	0.51
1:E:85:THR:HG22	1:E:86:PHE:CD2	2.45	0.51
1:H:222:ASP:OD1	1:H:224:THR:HG23	2.11	0.51
1:E:106:ILE:O	1:E:110:LEU:HB2	2.11	0.51
1:E:323:GLN:HE21	1:H:250:THR:HG21	1.76	0.51
1:G:243:LYS:HE3	2:G:2299:HOH:O	2.11	0.51
1:H:219:LEU:CD2	1:H:220:PRO:HD2	2.41	0.51
1:A:323:GLN:HE21	1:D:250:THR:HG21	1.76	0.51
1:D:9:THR:OG1	1:D:243:LYS:HA	2.10	0.51
1:D:327:GLN:OE1	1:D:331:VAL:HB	2.11	0.51
1:A:24:GLU:OE1	1:A:321:ARG:NH1	2.44	0.51
1:F:323:GLN:HG3	1:F:325:ILE:CD1	2.41	0.51
1:H:74:LYS:CG	1:H:114:VAL:HG22	2.40	0.51
1:C:327:GLN:OE1	1:C:331:VAL:HB	2.10	0.50
1:E:72:ASN:HB3	1:E:74:LYS:N	2.25	0.50
1:F:301:ALA:HB3	1:G:331:VAL:HG21	1.94	0.50
1:G:6:ILE:HB	2:G:2159:HOH:O	2.11	0.50
1:H:94:LYS:HG3	2:H:584:HOH:O	2.11	0.50
1:A:168:LYS:HG3	2:A:615:HOH:O	2.12	0.50
1:B:219:LEU:CD2	1:B:220:PRO:HD2	2.41	0.50
1:B:327:GLN:OE1	1:B:331:VAL:HB	2.10	0.50
1:C:176:SER:HB3	1:C:177:PRO:HA	1.94	0.50
1:D:94:LYS:HG3	2:D:590:HOH:O	2.11	0.50
1:B:24:GLU:OE1	1:B:321:ARG:NH1	2.44	0.50
1:C:115:THR:HA	1:C:148:ASP:OD1	2.11	0.50
1:F:155:VAL:HB	1:F:166:HIS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:ALA:HB2	1:H:252:LEU:HD13	1.93	0.50
1:H:83:TYR:CZ	1:H:157:GLU:HG2	2.45	0.50
1:A:155:VAL:HG13	1:A:173:MET:HE3	1.93	0.50
1:B:9:THR:HG23	1:B:241:LYS:HD2	1.93	0.50
1:A:246:THR:O	1:A:250:THR:HG23	2.11	0.50
1:D:323:GLN:HG3	1:D:325:ILE:CD1	2.41	0.50
1:F:80:MET:HG3	1:F:106:ILE:HG12	1.93	0.50
1:F:327:GLN:OE1	1:F:331:VAL:HB	2.12	0.50
1:H:193:THR:HB	1:H:194:PRO:CD	2.42	0.50
1:H:323:GLN:HG3	1:H:325:ILE:HD11	1.93	0.50
1:E:9:THR:OG1	1:E:243:LYS:HA	2.11	0.50
1:F:155:VAL:HG22	1:F:173:MET:HE3	1.94	0.50
1:C:84:ALA:O	1:C:85:THR:CB	2.55	0.50
1:E:167:ARG:HH11	1:E:167:ARG:HG2	1.76	0.50
1:G:1:CYS:HB3	1:G:18:THR:O	2.12	0.50
1:A:243:LYS:HE3	2:A:490:HOH:O	2.12	0.50
1:D:167:ARG:HD2	2:D:611:HOH:O	2.10	0.50
1:E:327:GLN:OE1	1:E:331:VAL:HB	2.12	0.50
1:H:333:VAL:HG11	2:H:591:HOH:O	2.12	0.50
1:B:7:ARG:NH1	1:B:13:SER:OG	2.40	0.49
1:F:235:TRP:HE3	1:F:235:TRP:HA	1.77	0.49
1:F:250:THR:CG2	1:G:323:GLN:HE21	2.25	0.49
1:B:72:ASN:HB3	1:B:74:LYS:N	2.26	0.49
1:B:323:GLN:HG3	1:B:325:ILE:HD11	1.92	0.49
1:D:24:GLU:OE1	1:D:321:ARG:NH1	2.46	0.49
1:F:178:GLY:HA3	2:F:2098:HOH:O	2.11	0.49
1:F:239:THR:HG22	1:G:265:VAL:CG1	2.43	0.49
1:C:61:ASP:HB3	1:C:135:ILE:HD11	1.94	0.49
1:E:262:PRO:HB2	1:H:239:THR:CG2	2.42	0.49
1:F:235:TRP:HA	1:F:235:TRP:CE3	2.48	0.49
1:G:24:GLU:OE1	1:G:321:ARG:NH1	2.45	0.49
1:G:83:TYR:CZ	1:G:157:GLU:HG2	2.47	0.49
1:H:72:ASN:HB3	1:H:74:LYS:N	2.28	0.49
1:A:115:THR:HA	1:A:148:ASP:OD1	2.12	0.49
1:C:83:TYR:CE2	1:C:157:GLU:HG2	2.47	0.49
1:G:115:THR:HA	1:G:148:ASP:OD1	2.12	0.49
1:G:327:GLN:OE1	1:G:331:VAL:HB	2.12	0.49
1:H:24:GLU:OE1	1:H:321:ARG:NH1	2.46	0.49
1:B:155:VAL:HG22	1:B:173:MET:HE3	1.93	0.49
1:B:245:GLU:HB3	1:C:334:MET:O	2.12	0.49
1:C:333:VAL:HG11	2:C:572:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ARG:HD2	2:A:520:HOH:O	2.12	0.49
1:C:85:THR:HG22	1:C:86:PHE:CD2	2.48	0.49
1:E:205:LEU:HD12	1:F:170:ILE:CG2	2.43	0.49
1:F:24:GLU:OE1	1:F:321:ARG:NH1	2.46	0.48
1:G:12:LYS:HD3	1:G:245:GLU:HB2	1.94	0.48
1:B:263:LYS:HD2	1:B:294:TYR:CE2	2.48	0.48
1:D:222:ASP:OD1	1:D:224:THR:HG23	2.13	0.48
1:D:115:THR:HA	1:D:148:ASP:OD1	2.12	0.48
1:F:7:ARG:HD3	2:F:1976:HOH:O	2.11	0.48
1:F:245:GLU:OE2	1:F:290:TYR:OH	2.31	0.48
1:G:40:LEU:HD21	1:G:126:TYR:CE1	2.43	0.48
1:B:175:ASN:HB2	1:B:225:PRO:HB3	1.96	0.48
1:E:24:GLU:OE1	1:E:321:ARG:NH1	2.46	0.48
1:E:328:LEU:HD23	1:H:317:PHE:HB3	1.94	0.48
1:D:85:THR:HG22	1:D:86:PHE:CD2	2.49	0.48
1:E:39:ARG:NH1	1:E:63:THR:HG21	2.29	0.48
1:F:9:THR:HG23	1:F:241:LYS:HD2	1.95	0.48
1:F:263:LYS:HD2	1:F:294:TYR:CE2	2.48	0.48
1:H:176:SER:HB3	1:H:177:PRO:HA	1.96	0.48
1:A:72:ASN:HB3	1:A:74:LYS:N	2.28	0.48
1:C:73:GLU:O	1:C:287:LYS:HE2	2.13	0.48
1:C:219:LEU:CD2	1:C:220:PRO:HD2	2.43	0.48
1:E:246:THR:O	1:E:250:THR:HG23	2.14	0.48
1:F:127:THR:HG22	1:F:129:LEU:HD23	1.95	0.48
1:A:39:ARG:NH1	1:A:63:THR:HG21	2.28	0.48
1:G:95:LYS:H	1:G:95:LYS:CD	2.16	0.48
1:E:331:VAL:HA	1:H:303:SER:HB2	1.96	0.48
1:H:235:TRP:HA	1:H:235:TRP:CE3	2.49	0.48
1:B:167:ARG:HD2	2:B:542:HOH:O	2.13	0.48
1:E:167:ARG:HD2	2:E:1634:HOH:O	2.13	0.48
1:H:80:MET:HG3	1:H:106:ILE:HG12	1.96	0.48
1:F:169:THR:HB	1:F:179:TYR:CZ	2.48	0.47
1:G:155:VAL:HB	1:G:166:HIS:HB2	1.96	0.47
1:G:198:GLN:O	1:H:190:ILE:HD12	2.14	0.47
1:E:301:ALA:HB3	1:H:331:VAL:HG21	1.96	0.47
1:G:127:THR:HG22	1:G:129:LEU:HD23	1.96	0.47
1:H:55:VAL:CG1	1:H:304:LEU:HB2	2.44	0.47
1:C:216:GLY:O	1:C:217:LEU:C	2.54	0.47
1:A:167:ARG:HG2	1:A:167:ARG:HH11	1.79	0.47
2:A:635:HOH:O	1:D:212:GLN:HG3	2.14	0.47
1:C:127:THR:HG22	1:C:129:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:TYR:CE2	1:D:157:GLU:HG2	2.49	0.47
1:A:219:LEU:CD2	1:A:220:PRO:HD2	2.45	0.47
1:B:115:THR:HA	1:B:148:ASP:OD1	2.15	0.47
1:C:72:ASN:HB3	1:C:74:LYS:N	2.28	0.47
1:E:325:ILE:HD12	1:H:299:ILE:CG2	2.44	0.47
1:F:8:THR:OG1	1:F:12:LYS:HB2	2.14	0.47
1:G:4:LEU:HA	1:G:171:GLY:O	2.15	0.47
1:H:40:LEU:HD21	1:H:126:TYR:CE1	2.41	0.47
1:H:135:ILE:HG13	2:H:632:HOH:O	2.14	0.47
1:H:167:ARG:HD2	2:H:603:HOH:O	2.14	0.47
1:A:67:LEU:O	1:A:80:MET:HE2	2.15	0.47
1:D:84:ALA:O	1:D:85:THR:CB	2.61	0.47
1:D:323:GLN:HG3	1:D:325:ILE:HD11	1.96	0.47
2:E:1500:HOH:O	1:H:333:VAL:HA	2.13	0.47
1:F:101:ASN:OD1	1:F:103:VAL:HB	2.15	0.47
1:D:246:THR:O	1:D:250:THR:HG23	2.15	0.47
1:E:169:THR:HB	1:E:179:TYR:CZ	2.50	0.47
1:E:262:PRO:HB2	1:H:239:THR:HG22	1.96	0.47
1:G:167:ARG:HD2	2:G:2334:HOH:O	2.15	0.47
1:A:235:TRP:CE3	1:A:235:TRP:HA	2.50	0.47
1:B:333:VAL:HA	2:C:477:HOH:O	2.14	0.47
1:C:155:VAL:HB	1:C:166:HIS:HB2	1.96	0.47
1:G:72:ASN:HB3	1:G:74:LYS:N	2.28	0.47
1:B:231:ARG:HH11	1:B:231:ARG:HD3	1.51	0.46
1:C:263:LYS:HD2	1:C:294:TYR:CE2	2.51	0.46
1:F:246:THR:O	1:F:250:THR:HG23	2.15	0.46
1:H:106:ILE:O	1:H:110:LEU:HB2	2.15	0.46
1:D:167:ARG:O	1:D:168:LYS:C	2.58	0.46
1:G:167:ARG:HG2	1:G:167:ARG:HH11	1.80	0.46
1:H:263:LYS:HD2	1:H:294:TYR:CE2	2.50	0.46
1:B:298:ARG:HG3	1:C:298:ARG:HG3	1.97	0.46
1:G:155:VAL:HG13	1:G:173:MET:HE3	1.96	0.46
1:B:301:ALA:HB3	1:C:331:VAL:HG21	1.97	0.46
1:G:36:TYR:CE1	1:G:314:LEU:HD13	2.50	0.46
1:A:216:GLY:O	1:A:217:LEU:C	2.58	0.46
1:B:6:ILE:HB	2:B:410:HOH:O	2.15	0.46
1:H:156:ILE:HG12	1:H:165:ILE:CD1	2.46	0.46
1:H:246:THR:O	1:H:250:THR:HG23	2.14	0.46
1:D:156:ILE:HG12	1:D:165:ILE:CD1	2.46	0.46
1:E:193:THR:HB	1:E:194:PRO:CD	2.46	0.46
1:E:245:GLU:HB3	1:H:334:MET:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:THR:HG21	2:H:426:HOH:O	2.15	0.46
1:B:176:SER:HB3	1:B:177:PRO:HA	1.98	0.46
1:B:193:THR:HB	1:B:194:PRO:CD	2.45	0.46
1:B:246:THR:O	1:B:250:THR:HG23	2.16	0.46
1:F:115:THR:HB	2:F:1990:HOH:O	2.15	0.46
1:F:176:SER:HB3	1:F:177:PRO:HA	1.97	0.46
1:F:183:GLN:HB3	2:F:1569:HOH:O	2.16	0.46
1:A:323:GLN:HG3	1:A:325:ILE:HD11	1.97	0.46
2:B:437:HOH:O	1:C:333:VAL:HA	2.15	0.46
1:D:175:ASN:HB2	1:D:225:PRO:HB3	1.97	0.46
1:H:155:VAL:CG1	1:H:173:MET:HE3	2.43	0.46
1:C:6:ILE:HB	2:C:451:HOH:O	2.16	0.46
1:C:167:ARG:O	1:C:168:LYS:C	2.59	0.46
1:E:7:ARG:NH1	1:E:13:SER:OG	2.41	0.46
1:F:65:PRO:HG3	1:F:314:LEU:HD21	1.98	0.46
1:H:68:TYR:HA	1:H:80:MET:HE2	1.97	0.46
1:A:333:VAL:HG11	2:A:506:HOH:O	2.16	0.46
1:C:168:LYS:HG3	2:C:678:HOH:O	2.16	0.46
1:F:31:ILE:HD12	1:F:307:GLU:HG3	1.98	0.46
1:F:56:GLY:HA2	1:F:289:TYR:CE2	2.51	0.46
1:A:72:ASN:HD22	1:A:72:ASN:HA	1.37	0.45
1:A:193:THR:HB	1:A:194:PRO:CD	2.46	0.45
2:A:504:HOH:O	1:D:209:PRO:HG2	2.15	0.45
1:E:263:LYS:HE2	2:H:377:HOH:O	2.16	0.45
1:G:84:ALA:O	1:G:85:THR:CB	2.61	0.45
1:C:36:TYR:CE1	1:C:314:LEU:HD13	2.51	0.45
1:D:7:ARG:HB2	2:D:604:HOH:O	2.16	0.45
1:F:34:ARG:HG3	1:F:309:LEU:O	2.17	0.45
1:G:85:THR:HG22	1:G:86:PHE:CD2	2.51	0.45
1:G:106:ILE:O	1:G:110:LEU:HB2	2.16	0.45
1:H:55:VAL:HG11	1:H:304:LEU:HB2	1.98	0.45
1:D:9:THR:HG23	1:D:241:LYS:HD2	1.99	0.45
1:D:135:ILE:HG13	2:D:640:HOH:O	2.16	0.45
1:E:55:VAL:HG11	1:E:304:LEU:HB2	1.98	0.45
1:B:167:ARG:O	1:B:168:LYS:C	2.59	0.45
1:B:239:THR:CG2	1:C:262:PRO:HB2	2.47	0.45
1:B:72:ASN:O	1:B:287:LYS:HG2	2.16	0.45
1:B:265:VAL:CG1	1:C:239:THR:HG22	2.47	0.45
1:E:58:GLY:HA3	1:E:66:VAL:O	2.17	0.45
2:E:2520:HOH:O	1:H:212:GLN:HG3	2.16	0.45
1:G:9:THR:HG23	1:G:241:LYS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:ILE:HD13	1:H:14:LEU:HB2	1.99	0.45
1:A:73:GLU:O	1:A:287:LYS:HE2	2.17	0.45
1:B:84:ALA:O	1:B:85:THR:CB	2.61	0.45
1:C:235:TRP:HE3	1:C:235:TRP:HA	1.82	0.45
1:E:244:ASN:HB2	2:E:2770:HOH:O	2.16	0.45
1:F:16:ALA:HB2	1:F:252:LEU:HD13	1.99	0.45
1:F:54:PHE:CE1	1:F:67:LEU:HD13	2.39	0.45
1:G:323:GLN:HG3	1:G:325:ILE:CD1	2.46	0.45
1:E:65:PRO:HG3	1:E:314:LEU:HD21	1.97	0.45
1:F:156:ILE:HG12	1:F:165:ILE:CD1	2.46	0.45
1:H:155:VAL:HB	1:H:166:HIS:HB2	1.99	0.45
1:E:55:VAL:CG1	1:E:304:LEU:HB2	2.47	0.45
1:E:216:GLY:O	1:E:217:LEU:C	2.58	0.45
1:E:331:VAL:HG21	1:H:301:ALA:HB3	1.99	0.45
1:F:167:ARG:O	1:F:168:LYS:C	2.60	0.45
1:G:169:THR:HB	1:G:179:TYR:CZ	2.52	0.45
1:A:169:THR:HB	1:A:179:TYR:CZ	2.52	0.45
1:A:301:ALA:HB3	1:D:331:VAL:HG21	1.99	0.45
1:C:222:ASP:OD1	1:C:224:THR:HG23	2.17	0.45
1:F:72:ASN:O	1:F:287:LYS:HG2	2.17	0.45
1:G:36:TYR:CZ	1:G:314:LEU:HD13	2.52	0.45
1:A:80:MET:HG3	1:A:106:ILE:HG12	1.99	0.44
1:B:334:MET:O	1:C:245:GLU:HB3	2.17	0.44
1:C:235:TRP:HA	1:C:235:TRP:CE3	2.52	0.44
1:F:323:GLN:HE21	1:G:250:THR:CG2	2.30	0.44
1:B:83:TYR:CE2	1:B:157:GLU:HG2	2.53	0.44
2:E:1512:HOH:O	1:H:250:THR:HG21	2.18	0.44
1:C:106:ILE:O	1:C:110:LEU:HB2	2.16	0.44
1:D:193:THR:HB	1:D:194:PRO:CD	2.48	0.44
1:F:250:THR:HG21	2:G:2212:HOH:O	2.17	0.44
1:G:7:ARG:HD3	2:G:2326:HOH:O	2.17	0.44
1:H:127:THR:HG22	1:H:129:LEU:HD23	1.98	0.44
1:H:155:VAL:HG22	1:H:173:MET:HE3	1.98	0.44
1:H:174:THR:OG1	1:H:175:ASN:N	2.49	0.44
1:H:235:TRP:HA	1:H:235:TRP:HE3	1.83	0.44
1:E:167:ARG:O	1:E:168:LYS:C	2.60	0.44
1:E:168:LYS:HG3	2:E:2053:HOH:O	2.17	0.44
1:F:193:THR:CB	1:F:194:PRO:CD	2.95	0.44
1:G:263:LYS:HD2	1:G:294:TYR:CE2	2.52	0.44
1:H:167:ARG:O	1:H:168:LYS:C	2.60	0.44
1:H:168:LYS:HG3	2:H:411:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:TRP:HA	1:A:235:TRP:HE3	1.81	0.44
1:A:331:VAL:HG21	1:D:301:ALA:HB3	1.99	0.44
1:B:55:VAL:HG11	1:B:304:LEU:HB2	1.99	0.44
1:E:260:ASN:O	1:E:262:PRO:HD3	2.17	0.44
1:B:156:ILE:HG12	1:B:165:ILE:HD13	1.99	0.44
1:C:175:ASN:HB2	1:C:225:PRO:HB3	2.00	0.44
1:E:40:LEU:HD21	1:E:126:TYR:CE1	2.44	0.44
1:A:65:PRO:HG3	1:A:314:LEU:HD21	1.99	0.44
1:A:176:SER:HB3	1:A:177:PRO:HA	1.99	0.44
1:B:80:MET:HG3	1:B:106:ILE:HG12	2.00	0.44
1:C:39:ARG:NH1	1:C:63:THR:HG21	2.33	0.44
1:C:245:GLU:OE2	1:C:290:TYR:OH	2.30	0.44
1:D:52:TYR:CE1	1:D:74:LYS:HD3	2.53	0.44
1:D:65:PRO:HG3	1:D:314:LEU:HD21	1.99	0.44
1:G:178:GLY:HA3	2:G:2448:HOH:O	2.17	0.44
1:D:52:TYR:CD1	1:D:74:LYS:HD3	2.53	0.44
1:F:244:ASN:HB2	2:G:2420:HOH:O	2.17	0.44
1:F:334:MET:O	1:G:245:GLU:HB3	2.18	0.44
1:G:222:ASP:OD1	1:G:224:THR:HG23	2.18	0.44
1:A:212:GLN:HG3	2:D:340:HOH:O	2.17	0.44
1:C:169:THR:HB	1:C:179:TYR:CZ	2.52	0.44
1:H:4:LEU:HA	1:H:171:GLY:O	2.18	0.44
1:B:55:VAL:CG1	1:B:304:LEU:HB2	2.47	0.43
1:C:148:ASP:HB3	1:C:150:SER:H	1.83	0.43
1:D:68:TYR:HA	1:D:80:MET:HE2	2.00	0.43
1:E:84:ALA:O	1:E:85:THR:CB	2.59	0.43
1:E:253:PHE:CE1	1:E:279:THR:HG22	2.53	0.43
1:G:83:TYR:CE2	1:G:157:GLU:HG2	2.52	0.43
1:G:231:ARG:HH11	1:G:231:ARG:HD3	1.58	0.43
1:A:155:VAL:HB	1:A:166:HIS:HB2	2.00	0.43
2:A:575:HOH:O	1:D:328:LEU:HG	2.18	0.43
1:G:333:VAL:HG11	2:G:2317:HOH:O	2.18	0.43
1:B:155:VAL:HB	1:B:166:HIS:HB2	1.99	0.43
1:B:224:THR:O	1:B:228:ARG:HG3	2.18	0.43
1:E:332:ASN:O	1:E:333:VAL:C	2.62	0.43
1:B:83:TYR:CZ	1:B:157:GLU:HG2	2.53	0.43
1:E:17:ARG:HD3	1:E:17:ARG:C	2.43	0.43
1:E:148:ASP:HB3	1:E:150:SER:H	1.83	0.43
1:F:17:ARG:HD2	1:F:69:ASP:OD2	2.18	0.43
1:F:168:LYS:HG3	2:F:1703:HOH:O	2.17	0.43
1:A:17:ARG:HD2	1:A:69:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ILE:HD12	1:C:252:LEU:HG	2.01	0.43
1:C:36:TYR:CZ	1:C:314:LEU:HD13	2.53	0.43
1:H:6:ILE:CD1	1:H:14:LEU:HB2	2.48	0.43
1:H:36:TYR:CZ	1:H:314:LEU:HD13	2.53	0.43
1:H:68:TYR:HA	1:H:80:MET:CE	2.48	0.43
1:F:109:VAL:HG11	1:F:146:PHE:CE1	2.53	0.43
1:G:176:SER:HB3	1:G:177:PRO:HA	2.00	0.43
1:D:245:GLU:OE2	1:D:290:TYR:OH	2.36	0.43
1:F:6:ILE:HD12	1:F:252:LEU:HG	2.00	0.43
1:F:323:GLN:HG3	1:F:325:ILE:HD11	2.00	0.43
1:G:332:ASN:O	1:G:333:VAL:C	2.61	0.43
1:A:83:TYR:CE2	1:A:157:GLU:HG2	2.54	0.43
1:A:4:LEU:HA	1:A:171:GLY:O	2.19	0.43
1:D:36:TYR:CE1	1:D:314:LEU:HD13	2.53	0.43
1:D:169:THR:HB	1:D:179:TYR:CZ	2.54	0.43
1:D:219:LEU:CD2	1:D:220:PRO:HD2	2.49	0.43
1:E:291:PHE:HE2	1:E:293:LEU:HD21	1.84	0.43
1:F:40:LEU:HD21	1:F:126:TYR:CE1	2.48	0.43
1:G:109:VAL:HG11	1:G:146:PHE:CE1	2.54	0.43
1:F:155:VAL:HG13	1:F:173:MET:HE3	2.00	0.42
1:F:212:GLN:HG3	2:G:1820:HOH:O	2.18	0.42
1:A:323:GLN:HG3	1:A:325:ILE:HD13	2.01	0.42
1:B:17:ARG:HD2	1:B:69:ASP:OD2	2.19	0.42
1:E:210:PHE:CE1	1:F:187:ARG:HB2	2.55	0.42
1:E:333:VAL:HG11	2:E:1617:HOH:O	2.19	0.42
1:H:39:ARG:NH1	1:H:63:THR:HG21	2.35	0.42
1:A:135:ILE:HG13	2:A:548:HOH:O	2.18	0.42
1:G:167:ARG:O	1:G:168:LYS:C	2.62	0.42
1:B:67:LEU:O	1:B:80:MET:HE2	2.20	0.42
1:B:169:THR:HB	1:B:179:TYR:CZ	2.54	0.42
1:C:58:GLY:HA3	1:C:66:VAL:O	2.20	0.42
1:G:94:LYS:HG3	2:G:2309:HOH:O	2.19	0.42
2:E:1615:HOH:O	1:H:209:PRO:HG2	2.19	0.42
1:F:135:ILE:HG13	2:F:2019:HOH:O	2.19	0.42
1:A:156:ILE:HG12	1:A:165:ILE:CD1	2.50	0.42
1:B:36:TYR:CZ	1:B:314:LEU:HD13	2.55	0.42
1:C:67:LEU:O	1:C:80:MET:HE2	2.20	0.42
1:C:332:ASN:O	1:C:333:VAL:C	2.63	0.42
1:D:73:GLU:O	1:D:287:LYS:HE2	2.19	0.42
1:G:175:ASN:HB2	1:G:225:PRO:HB3	2.01	0.42
1:E:83:TYR:CD2	1:E:143:HIS:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:ASN:HB2	2:H:362:HOH:O	2.20	0.42
1:F:143:HIS:HB2	1:F:157:GLU:HG3	2.01	0.42
1:A:167:ARG:O	1:A:168:LYS:C	2.62	0.42
1:B:263:LYS:HE3	1:B:275:TYR:CE2	2.54	0.42
1:C:332:ASN:HB2	2:C:556:HOH:O	2.19	0.42
1:D:155:VAL:HB	1:D:166:HIS:HB2	2.02	0.42
1:F:29:VAL:HG13	1:F:317:PHE:HB2	2.02	0.42
1:G:67:LEU:O	1:G:80:MET:HE2	2.19	0.42
1:C:244:ASN:HB2	2:C:391:HOH:O	2.18	0.42
1:G:156:ILE:HG12	1:G:165:ILE:CD1	2.50	0.42
1:H:193:THR:HB	1:H:194:PRO:HD2	2.01	0.42
1:A:9:THR:HG23	1:A:241:LYS:HD2	2.02	0.42
1:A:72:ASN:O	1:A:287:LYS:HG2	2.20	0.42
1:B:193:THR:CB	1:B:194:PRO:CD	2.98	0.42
1:B:308:ASN:O	1:B:311:SER:OG	2.38	0.42
1:H:17:ARG:HH11	1:H:69:ASP:HB3	1.85	0.42
1:F:298:ARG:HG3	1:G:298:ARG:HG3	2.02	0.41
1:F:323:GLN:HG3	1:F:325:ILE:HD13	2.02	0.41
2:F:2413:HOH:O	1:G:263:LYS:HE2	2.19	0.41
1:H:155:VAL:HG11	1:H:179:TYR:HB2	2.02	0.41
1:H:185:ASN:O	1:H:186:LEU:C	2.63	0.41
1:A:7:ARG:HD3	2:A:513:HOH:O	2.20	0.41
1:A:175:ASN:HB2	1:A:225:PRO:HB3	2.02	0.41
1:B:106:ILE:O	1:B:110:LEU:HB2	2.19	0.41
1:B:222:ASP:OD1	1:B:224:THR:HG23	2.20	0.41
1:E:73:GLU:O	1:E:287:LYS:HE2	2.20	0.41
1:F:332:ASN:O	1:F:333:VAL:C	2.64	0.41
1:H:29:VAL:HG13	1:H:317:PHE:HB2	2.01	0.41
1:B:328:LEU:HD22	1:C:302:VAL:HG23	2.02	0.41
1:D:178:GLY:HA3	2:D:689:HOH:O	2.20	0.41
1:E:185:ASN:O	1:E:186:LEU:C	2.63	0.41
1:H:166:HIS:CD2	1:H:179:TYR:HB3	2.55	0.41
1:H:291:PHE:HE2	1:H:293:LEU:HD21	1.86	0.41
1:D:235:TRP:HA	1:D:235:TRP:CE3	2.55	0.41
1:F:198:GLN:HB2	2:F:1524:HOH:O	2.20	0.41
1:H:260:ASN:O	1:H:262:PRO:HD3	2.21	0.41
1:B:245:GLU:OE2	1:B:290:TYR:OH	2.35	0.41
1:E:328:LEU:HD22	1:H:302:VAL:HG23	2.03	0.41
1:G:65:PRO:HG3	1:G:314:LEU:HD21	2.02	0.41
1:G:72:ASN:O	1:G:287:LYS:HG2	2.21	0.41
1:H:7:ARG:HD3	2:H:596:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:THR:HG22	1:B:86:PHE:CD2	2.55	0.41
1:C:65:PRO:HG3	1:C:314:LEU:HD21	2.03	0.41
1:E:52:TYR:CE1	1:E:74:LYS:HD3	2.55	0.41
1:G:7:ARG:NH1	1:G:13:SER:OG	2.47	0.41
1:G:55:VAL:CG1	1:G:304:LEU:HB2	2.51	0.41
1:A:83:TYR:CZ	1:A:157:GLU:HG2	2.56	0.41
1:A:84:ALA:O	1:A:85:THR:CB	2.58	0.41
1:A:239:THR:HG22	1:D:262:PRO:HB2	2.02	0.41
1:B:69:ASP:HA	1:B:78:GLY:O	2.21	0.41
1:F:52:TYR:CD1	1:F:74:LYS:HD3	2.56	0.41
1:G:219:LEU:CD2	1:G:220:PRO:HD2	2.49	0.41
1:H:29:VAL:HG22	1:H:317:PHE:HD1	1.86	0.41
1:A:332:ASN:O	1:A:333:VAL:C	2.63	0.41
1:B:34:ARG:HG3	1:B:309:LEU:O	2.20	0.41
1:C:10:ASP:OD2	1:C:12:LYS:HD2	2.21	0.41
1:D:6:ILE:HB	2:D:475:HOH:O	2.20	0.41
1:D:72:ASN:HB3	1:D:74:LYS:N	2.36	0.41
1:F:323:GLN:HE21	1:G:250:THR:HG21	1.85	0.41
1:G:17:ARG:HD3	1:G:17:ARG:C	2.46	0.41
1:A:219:LEU:HD12	1:A:235:TRP:CZ2	2.55	0.41
1:A:245:GLU:OE2	1:A:290:TYR:OH	2.35	0.41
1:C:193:THR:HB	1:C:194:PRO:HD2	2.01	0.41
1:D:40:LEU:HD21	1:D:126:TYR:CE1	2.44	0.41
1:E:166:HIS:CD2	1:E:179:TYR:HB3	2.55	0.41
1:E:175:ASN:HB2	1:E:225:PRO:HB3	2.03	0.41
1:F:260:ASN:O	1:F:262:PRO:HD3	2.21	0.41
1:F:291:PHE:HE2	1:F:293:LEU:HD21	1.86	0.41
1:G:110:LEU:HD12	1:G:110:LEU:HA	1.95	0.41
1:H:36:TYR:CE1	1:H:314:LEU:HD13	2.56	0.41
1:A:334:MET:O	1:D:245:GLU:HB3	2.21	0.41
1:E:9:THR:HG23	1:E:241:LYS:HD2	2.03	0.41
1:E:52:TYR:CD1	1:E:74:LYS:HD3	2.56	0.41
1:F:106:ILE:O	1:F:110:LEU:HB2	2.21	0.41
1:G:16:ALA:HB2	1:G:252:LEU:HD13	2.03	0.41
1:B:72:ASN:HB2	1:B:76:LEU:H	1.86	0.40
1:B:235:TRP:HA	1:B:235:TRP:CE3	2.56	0.40
1:C:17:ARG:HD3	1:C:17:ARG:C	2.46	0.40
1:F:36:TYR:CZ	1:F:314:LEU:HD13	2.56	0.40
1:G:55:VAL:HG11	1:G:304:LEU:HB2	2.03	0.40
1:H:109:VAL:HG11	1:H:146:PHE:CE1	2.56	0.40
1:H:183:GLN:HB3	2:H:404:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:322:LYS:HB3	2:H:637:HOH:O	2.20	0.40
1:C:185:ASN:O	1:C:186:LEU:C	2.65	0.40
1:F:308:ASN:O	1:F:311:SER:OG	2.38	0.40
1:G:174:THR:OG1	1:G:175:ASN:N	2.54	0.40
1:G:235:TRP:HA	1:G:235:TRP:CE3	2.56	0.40
1:H:109:VAL:HG13	1:H:119:VAL:HG22	2.03	0.40
1:B:331:VAL:HG21	1:C:301:ALA:HB3	2.03	0.40
1:F:174:THR:OG1	1:F:175:ASN:N	2.54	0.40
1:G:235:TRP:HA	1:G:235:TRP:HE3	1.87	0.40
1:H:72:ASN:HD22	1:H:72:ASN:HA	1.35	0.40
1:A:106:ILE:O	1:A:110:LEU:HB2	2.21	0.40
1:B:156:ILE:HG12	1:B:165:ILE:CD1	2.51	0.40
1:B:268:THR:HA	1:C:212:GLN:NE2	2.37	0.40
1:D:231:ARG:HH11	1:D:231:ARG:HD3	1.64	0.40
1:E:67:LEU:O	1:E:80:MET:HE2	2.21	0.40
1:F:166:HIS:CD2	1:F:179:TYR:HB3	2.56	0.40
1:A:296:ASN:ND2	1:A:324:ASP:H	2.19	0.40
1:B:135:ILE:HG13	2:B:571:HOH:O	2.21	0.40
1:C:34:ARG:HG3	1:C:309:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/335 (99%)	317 (96%)	13 (4%)	2 (1%)	21	51
1	B	332/335 (99%)	318 (96%)	12 (4%)	2 (1%)	21	51
1	C	332/335 (99%)	317 (96%)	13 (4%)	2 (1%)	21	51
1	D	332/335 (99%)	317 (96%)	13 (4%)	2 (1%)	21	51
1	E	332/335 (99%)	316 (95%)	14 (4%)	2 (1%)	21	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	F	332/335 (99%)	317 (96%)	13 (4%)	2 (1%)	21	51	
1	G	332/335 (99%)	317 (96%)	13 (4%)	2 (1%)	21	51	
1	H	332/335 (99%)	314 (95%)	16 (5%)	2 (1%)	21	51	
All	All	2656/2680 (99%)	2533 (95%)	107 (4%)	16 (1%)	21	51	

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	VAL
1	B	168	LYS
1	C	168	LYS
1	D	168	LYS
1	E	333	VAL
1	G	333	VAL
1	H	168	LYS
1	C	333	VAL
1	D	333	VAL
1	E	168	LYS
1	F	168	LYS
1	F	333	VAL
1	G	168	LYS
1	A	168	LYS
1	B	333	VAL
1	H	333	VAL

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	291/292 (100%)	234 (80%)	57 (20%)	1	5	
1	B	291/292 (100%)	235 (81%)	56 (19%)	1	5	
1	C	291/292 (100%)	236 (81%)	55 (19%)	1	5	
1	D	291/292 (100%)	234 (80%)	57 (20%)	1	5	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	291/292 (100%)	233 (80%)	58 (20%)	1	5
1	F	291/292 (100%)	232 (80%)	59 (20%)	1	4
1	G	291/292 (100%)	232 (80%)	59 (20%)	1	4
1	H	291/292 (100%)	233 (80%)	58 (20%)	1	5
All	All	2328/2336 (100%)	1869 (80%)	459 (20%)	1	5

All (459) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	4	LEU
1	A	6	ILE
1	A	10	ASP
1	A	23	MET
1	A	26	ASP
1	A	28	LYS
1	A	29	VAL
1	A	34	ARG
1	A	40	LEU
1	A	41	LEU
1	A	67	LEU
1	A	71	VAL
1	A	72	ASN
1	A	74	LYS
1	A	82	TYR
1	A	85	THR
1	A	94	LYS
1	A	95	LYS
1	A	98	THR
1	A	103	VAL
1	A	110	LEU
1	A	121	GLU
1	A	123	LEU
1	A	130	ASN
1	A	134	ILE
1	A	136	LEU
1	A	142	LEU
1	A	152	GLU
1	A	160	LYS
1	A	167	ARG
1	A	168	LYS

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Mol	Chain	Res	Type
1	A	173	MET
1	A	180	GLU
1	A	205	LEU
1	A	208	THR
1	A	212	GLN
1	A	219	LEU
1	A	230	LEU
1	A	241	LYS
1	A	243	LYS
1	A	250	THR
1	A	265	VAL
1	A	269	ASN
1	A	270	GLU
1	A	272	LYS
1	A	273	THR
1	A	285	GLN
1	A	293	LEU
1	A	305	MET
1	A	311	SER
1	A	314	LEU
1	A	318	GLU
1	A	321	ARG
1	A	327	GLN
1	A	330	GLN
1	A	334	MET
1	B	1	CYS
1	B	6	ILE
1	B	10	ASP
1	B	23	MET
1	B	26	ASP
1	B	28	LYS
1	B	29	VAL
1	B	31	ILE
1	B	34	ARG
1	B	40	LEU
1	B	41	LEU
1	B	67	LEU
1	B	71	VAL
1	B	72	ASN
1	B	74	LYS
1	B	82	TYR
1	B	85	THR

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Mol	Chain	Res	Type
1	B	94	LYS
1	B	95	LYS
1	B	98	THR
1	B	103	VAL
1	B	110	LEU
1	B	121	GLU
1	B	123	LEU
1	B	130	ASN
1	B	134	ILE
1	B	136	LEU
1	B	142	LEU
1	B	152	GLU
1	B	160	LYS
1	B	167	ARG
1	B	168	LYS
1	B	173	MET
1	B	180	GLU
1	B	205	LEU
1	B	208	THR
1	B	212	GLN
1	B	219	LEU
1	B	230	LEU
1	B	241	LYS
1	B	243	LYS
1	B	250	THR
1	B	265	VAL
1	B	269	ASN
1	B	270	GLU
1	B	272	LYS
1	B	273	THR
1	B	285	GLN
1	B	293	LEU
1	B	311	SER
1	B	314	LEU
1	B	318	GLU
1	B	321	ARG
1	B	327	GLN
1	B	330	GLN
1	B	334	MET
1	C	1	CYS
1	C	6	ILE
1	C	10	ASP

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Mol	Chain	Res	Type
1	C	23	MET
1	C	26	ASP
1	C	28	LYS
1	C	29	VAL
1	C	34	ARG
1	C	41	LEU
1	C	67	LEU
1	C	71	VAL
1	C	72	ASN
1	C	74	LYS
1	C	82	TYR
1	C	85	THR
1	C	94	LYS
1	C	95	LYS
1	C	98	THR
1	C	103	VAL
1	C	110	LEU
1	C	121	GLU
1	C	123	LEU
1	C	130	ASN
1	C	134	ILE
1	C	136	LEU
1	C	142	LEU
1	C	152	GLU
1	C	160	LYS
1	C	167	ARG
1	C	168	LYS
1	C	173	MET
1	C	180	GLU
1	C	205	LEU
1	C	208	THR
1	C	212	GLN
1	C	219	LEU
1	C	230	LEU
1	C	241	LYS
1	C	243	LYS
1	C	250	THR
1	C	265	VAL
1	C	269	ASN
1	C	270	GLU
1	C	272	LYS
1	C	273	THR

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Mol	Chain	Res	Type
1	C	285	GLN
1	C	293	LEU
1	C	305	MET
1	C	311	SER
1	C	314	LEU
1	C	318	GLU
1	C	321	ARG
1	C	327	GLN
1	C	330	GLN
1	C	334	MET
1	D	1	CYS
1	D	6	ILE
1	D	10	ASP
1	D	23	MET
1	D	26	ASP
1	D	27	SER
1	D	28	LYS
1	D	29	VAL
1	D	34	ARG
1	D	40	LEU
1	D	41	LEU
1	D	67	LEU
1	D	71	VAL
1	D	72	ASN
1	D	74	LYS
1	D	82	TYR
1	D	85	THR
1	D	94	LYS
1	D	95	LYS
1	D	98	THR
1	D	103	VAL
1	D	110	LEU
1	D	121	GLU
1	D	123	LEU
1	D	130	ASN
1	D	134	ILE
1	D	136	LEU
1	D	142	LEU
1	D	152	GLU
1	D	160	LYS
1	D	167	ARG
1	D	168	LYS

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Mol	Chain	Res	Type
1	D	173	MET
1	D	180	GLU
1	D	205	LEU
1	D	208	THR
1	D	212	GLN
1	D	219	LEU
1	D	230	LEU
1	D	235	TRP
1	D	241	LYS
1	D	243	LYS
1	D	250	THR
1	D	265	VAL
1	D	269	ASN
1	D	270	GLU
1	D	272	LYS
1	D	273	THR
1	D	285	GLN
1	D	293	LEU
1	D	311	SER
1	D	314	LEU
1	D	318	GLU
1	D	321	ARG
1	D	327	GLN
1	D	330	GLN
1	D	334	MET
1	E	1	CYS
1	E	4	LEU
1	E	6	ILE
1	E	10	ASP
1	E	23	MET
1	E	26	ASP
1	E	28	LYS
1	E	29	VAL
1	E	34	ARG
1	E	40	LEU
1	E	41	LEU
1	E	67	LEU
1	E	71	VAL
1	E	72	ASN
1	E	74	LYS
1	E	82	TYR
1	E	85	THR

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Mol	Chain	Res	Type
1	E	94	LYS
1	E	95	LYS
1	E	98	THR
1	E	103	VAL
1	E	110	LEU
1	E	121	GLU
1	E	123	LEU
1	E	130	ASN
1	E	134	ILE
1	E	136	LEU
1	E	142	LEU
1	E	145	THR
1	E	152	GLU
1	E	160	LYS
1	E	167	ARG
1	E	168	LYS
1	E	173	MET
1	E	180	GLU
1	E	205	LEU
1	E	212	GLN
1	E	219	LEU
1	E	230	LEU
1	E	235	TRP
1	E	241	LYS
1	E	243	LYS
1	E	250	THR
1	E	265	VAL
1	E	269	ASN
1	E	270	GLU
1	E	272	LYS
1	E	273	THR
1	E	285	GLN
1	E	293	LEU
1	E	305	MET
1	E	311	SER
1	E	314	LEU
1	E	318	GLU
1	E	321	ARG
1	E	327	GLN
1	E	330	GLN
1	E	334	MET
1	F	1	CYS

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Mol	Chain	Res	Type
1	F	4	LEU
1	F	6	ILE
1	F	10	ASP
1	F	23	MET
1	F	26	ASP
1	F	28	LYS
1	F	29	VAL
1	F	31	ILE
1	F	34	ARG
1	F	41	LEU
1	F	67	LEU
1	F	71	VAL
1	F	72	ASN
1	F	74	LYS
1	F	82	TYR
1	F	85	THR
1	F	94	LYS
1	F	95	LYS
1	F	98	THR
1	F	103	VAL
1	F	110	LEU
1	F	121	GLU
1	F	123	LEU
1	F	130	ASN
1	F	134	ILE
1	F	136	LEU
1	F	142	LEU
1	F	152	GLU
1	F	160	LYS
1	F	167	ARG
1	F	168	LYS
1	F	173	MET
1	F	180	GLU
1	F	205	LEU
1	F	208	THR
1	F	212	GLN
1	F	219	LEU
1	F	230	LEU
1	F	241	LYS
1	F	243	LYS
1	F	250	THR
1	F	265	VAL

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Mol	Chain	Res	Type
1	F	269	ASN
1	F	270	GLU
1	F	272	LYS
1	F	273	THR
1	F	282	MET
1	F	285	GLN
1	F	292	LYS
1	F	293	LEU
1	F	305	MET
1	F	311	SER
1	F	314	LEU
1	F	318	GLU
1	F	321	ARG
1	F	327	GLN
1	F	330	GLN
1	F	334	MET
1	G	1	CYS
1	G	4	LEU
1	G	6	ILE
1	G	10	ASP
1	G	23	MET
1	G	26	ASP
1	G	28	LYS
1	G	29	VAL
1	G	34	ARG
1	G	40	LEU
1	G	41	LEU
1	G	67	LEU
1	G	71	VAL
1	G	72	ASN
1	G	74	LYS
1	G	82	TYR
1	G	85	THR
1	G	94	LYS
1	G	95	LYS
1	G	98	THR
1	G	103	VAL
1	G	110	LEU
1	G	121	GLU
1	G	123	LEU
1	G	130	ASN
1	G	134	ILE

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Mol	Chain	Res	Type
1	G	136	LEU
1	G	142	LEU
1	G	145	THR
1	G	152	GLU
1	G	160	LYS
1	G	167	ARG
1	G	168	LYS
1	G	173	MET
1	G	180	GLU
1	G	205	LEU
1	G	208	THR
1	G	212	GLN
1	G	219	LEU
1	G	230	LEU
1	G	235	TRP
1	G	241	LYS
1	G	243	LYS
1	G	250	THR
1	G	265	VAL
1	G	269	ASN
1	G	270	GLU
1	G	272	LYS
1	G	273	THR
1	G	282	MET
1	G	285	GLN
1	G	293	LEU
1	G	311	SER
1	G	314	LEU
1	G	318	GLU
1	G	321	ARG
1	G	327	GLN
1	G	330	GLN
1	G	334	MET
1	H	6	ILE
1	H	10	ASP
1	H	23	MET
1	H	26	ASP
1	H	28	LYS
1	H	29	VAL
1	H	31	ILE
1	H	34	ARG
1	H	40	LEU

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Mol	Chain	Res	Type
1	H	41	LEU
1	H	67	LEU
1	H	71	VAL
1	H	72	ASN
1	H	74	LYS
1	H	82	TYR
1	H	85	THR
1	H	94	LYS
1	H	95	LYS
1	H	98	THR
1	H	103	VAL
1	H	110	LEU
1	H	121	GLU
1	H	123	LEU
1	H	130	ASN
1	H	134	ILE
1	H	136	LEU
1	H	142	LEU
1	H	152	GLU
1	H	160	LYS
1	H	167	ARG
1	H	168	LYS
1	H	173	MET
1	H	180	GLU
1	H	205	LEU
1	H	208	THR
1	H	212	GLN
1	H	219	LEU
1	H	230	LEU
1	H	235	TRP
1	H	241	LYS
1	H	243	LYS
1	H	250	THR
1	H	265	VAL
1	H	269	ASN
1	H	270	GLU
1	H	272	LYS
1	H	273	THR
1	H	282	MET
1	H	285	GLN
1	H	293	LEU
1	H	305	MET

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Mol	Chain	Res	Type
1	H	311	SER
1	H	314	LEU
1	H	318	GLU
1	H	321	ARG
1	H	327	GLN
1	H	330	GLN
1	H	334	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	49	ASN
1	A	72	ASN
1	A	130	ASN
1	A	133	ASN
1	A	166	HIS
1	A	182	HIS
1	A	185	ASN
1	A	251	ASN
1	A	269	ASN
1	A	288	ASN
1	A	296	ASN
1	A	308	ASN
1	B	35	ASN
1	B	49	ASN
1	B	72	ASN
1	B	130	ASN
1	B	133	ASN
1	B	166	HIS
1	B	182	HIS
1	B	185	ASN
1	B	251	ASN
1	B	269	ASN
1	B	288	ASN
1	B	296	ASN
1	B	308	ASN
1	C	35	ASN
1	C	49	ASN
1	C	72	ASN
1	C	130	ASN
1	C	133	ASN

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Mol	Chain	Res	Type
1	C	166	HIS
1	C	185	ASN
1	C	212	GLN
1	C	251	ASN
1	C	269	ASN
1	C	288	ASN
1	C	308	ASN
1	D	72	ASN
1	D	130	ASN
1	D	133	ASN
1	D	166	HIS
1	D	182	HIS
1	D	185	ASN
1	D	212	GLN
1	D	251	ASN
1	D	269	ASN
1	D	288	ASN
1	D	296	ASN
1	D	308	ASN
1	E	35	ASN
1	E	49	ASN
1	E	72	ASN
1	E	130	ASN
1	E	133	ASN
1	E	166	HIS
1	E	182	HIS
1	E	185	ASN
1	E	212	GLN
1	E	251	ASN
1	E	269	ASN
1	E	288	ASN
1	E	296	ASN
1	E	308	ASN
1	F	35	ASN
1	F	49	ASN
1	F	130	ASN
1	F	133	ASN
1	F	166	HIS
1	F	182	HIS
1	F	185	ASN
1	F	212	GLN
1	F	251	ASN

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Mol	Chain	Res	Type
1	F	254	HIS
1	F	269	ASN
1	F	288	ASN
1	F	296	ASN
1	F	308	ASN
1	G	72	ASN
1	G	130	ASN
1	G	133	ASN
1	G	166	HIS
1	G	182	HIS
1	G	185	ASN
1	G	251	ASN
1	G	260	ASN
1	G	269	ASN
1	G	296	ASN
1	G	308	ASN
1	H	72	ASN
1	H	130	ASN
1	H	133	ASN
1	H	166	HIS
1	H	182	HIS
1	H	185	ASN
1	H	251	ASN
1	H	260	ASN
1	H	269	ASN
1	H	308	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.