



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:35 AM UTC

PDB ID : 1DT5 / pdb_00001dt5
Title : THE STRUCTURAL ORIGINS OF INTERFACIAL ACTIVATION IN THERMOMYCES (HUMICOLA) LANUGINOSA LIPASE
Authors : Brozozowski, A.M.; Savage, H.
Deposited on : 2000-01-11
Resolution : 2.40 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

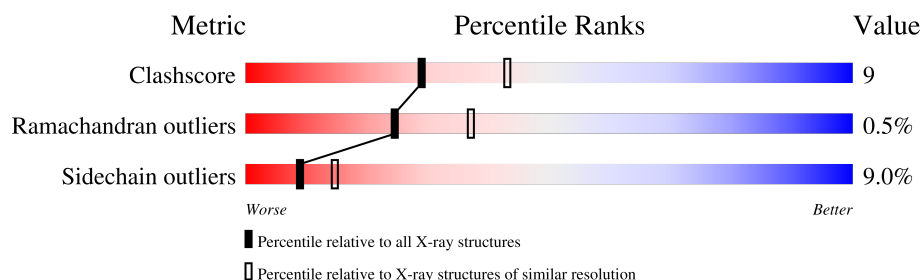
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	269	69% 23% 7% .
1	B	269	70% 23% 6% .
1	C	269	74% 19% 6% .
1	D	269	70% 20% 7% .
1	E	269	71% 22% 6% .
1	F	269	68% 27% . .
1	G	269	67% 27% . .
1	H	269	71% 23% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17081 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 LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	B	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	C	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	D	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	E	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	F	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	G	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			
1	H	269	Total	C	N	O	S	0	0	0
			2071	1303	359	403	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	0	0
			90	90		
2	B	102	Total	O	0	0
			102	102		
2	C	64	Total	O	0	0
			64	64		
2	D	68	Total	O	0	0
			68	68		
2	E	57	Total	O	0	0
			57	57		
2	F	51	Total	O	0	0
			51	51		

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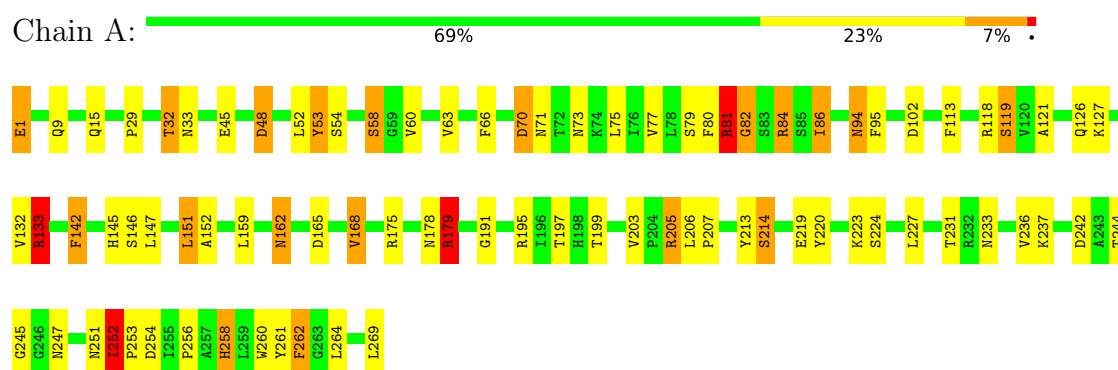
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	30	Total 30	O 30	0	0
2	H	51	Total 51	O 51	0	0

3 Residue-property plots

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.

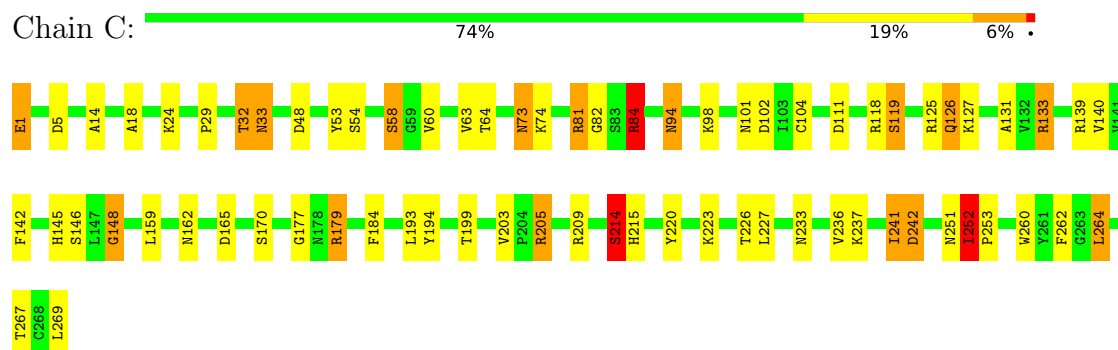
• Molecule 1: LIPASE



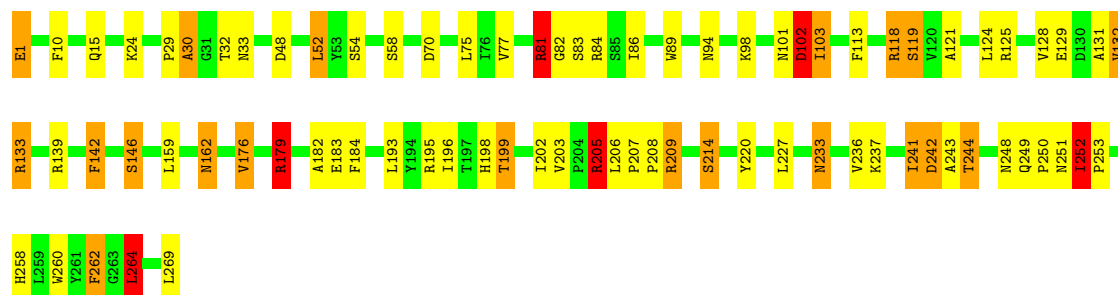
• Molecule 1: LIPASE



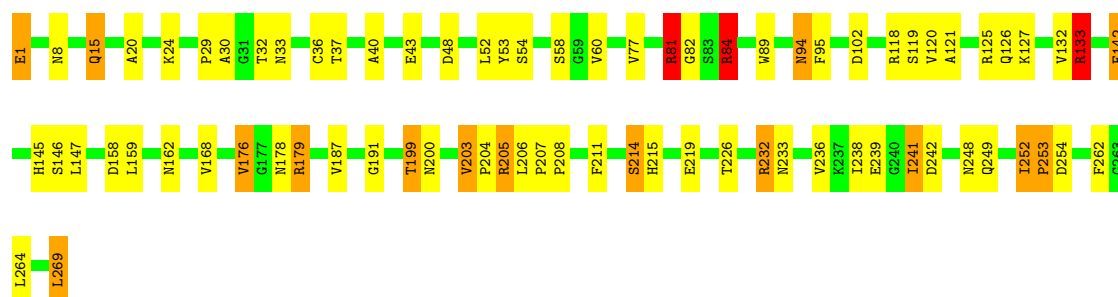
• Molecule 1: LIPASE



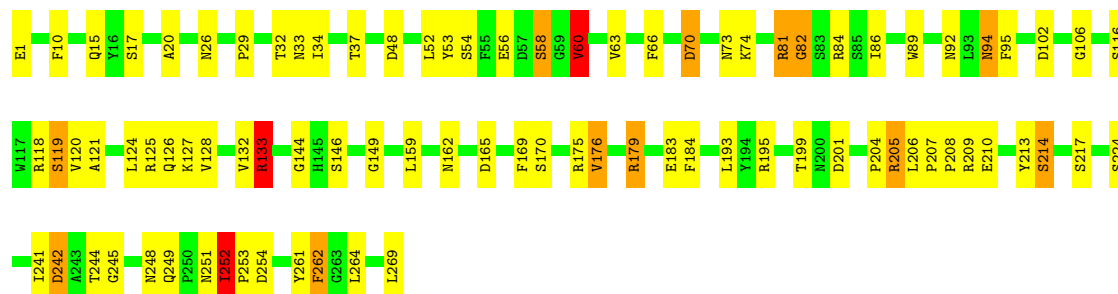
• Molecule 1: LIPASE

Chain D: 

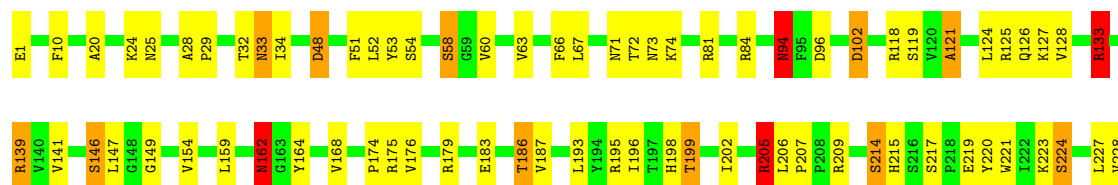
• Molecule 1: LIPASE

Chain E: 

• Molecule 1: LIPASE

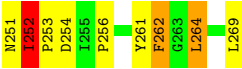
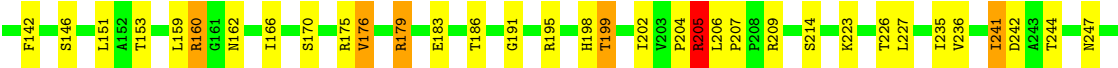
Chain F: 

• Molecule 1: LIPASE

Chain G: 



● Molecule 1: LIPASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.44Å 162.88Å 86.72Å 90.00° 98.45° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	98.4 (20.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.244 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17081	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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	0.85	2/2121 (0.1%)	1.97	71/2887 (2.5%)
1	B	0.87	2/2121 (0.1%)	2.04	61/2887 (2.1%)
1	C	0.71	0/2121	1.84	44/2887 (1.5%)
1	D	0.75	1/2121 (0.0%)	1.89	63/2887 (2.2%)
1	E	0.67	0/2121	1.77	35/2887 (1.2%)
1	F	0.71	0/2121	1.82	48/2887 (1.7%)
1	G	0.63	0/2121	1.70	30/2887 (1.0%)
1	H	0.68	0/2121	1.78	38/2887 (1.3%)
All	All	0.74	5/16968 (0.0%)	1.85	390/23096 (1.7%)

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	3
1	C	0	6
1	D	0	5
1	E	0	4
1	F	0	4
1	G	0	7
1	H	0	2
All	All	0	39

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	ARG	CD-NE	-6.67	1.36	1.46
1	A	245	GLY	N-CA	5.61	1.53	1.45
1	B	205	ARG	CD-NE	-5.49	1.38	1.46
1	D	205	ARG	CD-NE	-5.42	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	ARG	CD-NE	-5.05	1.39	1.46

All (390) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	ARG	CD-NE-CZ	24.60	158.84	124.40
1	H	205	ARG	CD-NE-CZ	23.46	157.25	124.40
1	D	205	ARG	CD-NE-CZ	20.63	153.28	124.40
1	A	205	ARG	CD-NE-CZ	19.73	152.03	124.40
1	B	48	ASP	CA-CB-CG	16.29	128.89	112.60
1	A	48	ASP	CA-CB-CG	16.03	128.63	112.60
1	C	205	ARG	CD-NE-CZ	14.05	144.07	124.40
1	E	249	GLN	OE1-CD-NE2	-13.98	108.62	122.60
1	C	48	ASP	CA-CB-CG	13.68	126.28	112.60
1	G	205	ARG	CD-NE-CZ	13.19	142.87	124.40
1	E	48	ASP	CA-CB-CG	13.19	125.79	112.60
1	F	205	ARG	CD-NE-CZ	13.12	142.77	124.40
1	E	205	ARG	CD-NE-CZ	11.72	140.81	124.40
1	A	244	THR	CA-C-N	-11.56	109.68	123.44
1	A	244	THR	C-N-CA	-11.56	109.68	123.44
1	F	48	ASP	CA-CB-CG	11.15	123.75	112.60
1	B	175	ARG	NE-CZ-NH2	11.12	129.21	119.20
1	D	48	ASP	CA-CB-CG	11.06	123.66	112.60
1	B	262	PHE	CA-C-N	10.96	136.12	120.56
1	B	262	PHE	C-N-CA	10.96	136.12	120.56
1	A	179	ARG	NE-CZ-NH2	10.61	128.75	119.20
1	E	205	ARG	NE-CZ-NH2	-10.13	110.08	119.20
1	G	48	ASP	CA-CB-CG	10.10	122.70	112.60
1	F	205	ARG	NE-CZ-NH1	9.50	131.00	121.50
1	C	126	GLN	CB-CG-CD	9.35	128.49	112.60
1	B	241	ILE	O-C-N	-9.31	113.76	122.79
1	G	60	VAL	N-CA-C	9.19	120.00	110.72
1	E	249	GLN	CG-CD-NE2	9.16	130.14	116.40
1	B	133	ARG	CD-NE-CZ	9.06	137.09	124.40
1	H	48	ASP	CA-CB-CG	8.95	121.55	112.60
1	A	81	ARG	NE-CZ-NH1	8.87	130.37	121.50
1	H	252	ILE	CB-CA-C	8.78	119.11	110.94
1	E	232	ARG	CD-NE-CZ	8.71	136.59	124.40
1	A	262	PHE	CA-C-N	8.68	134.07	120.97
1	A	262	PHE	C-N-CA	8.68	134.07	120.97
1	A	205	ARG	CG-CD-NE	8.67	131.07	112.00
1	G	133	ARG	CD-NE-CZ	8.62	136.47	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ARG	NE-CZ-NH1	8.56	130.06	121.50
1	D	202	ILE	CA-C-N	8.55	127.17	120.33
1	D	202	ILE	C-N-CA	8.55	127.17	120.33
1	A	133	ARG	CD-NE-CZ	8.48	136.28	124.40
1	F	133	ARG	CD-NE-CZ	8.47	136.25	124.40
1	C	205	ARG	CB-CG-CD	8.42	130.66	111.30
1	C	177	GLY	CA-C-O	8.34	130.14	121.21
1	H	133	ARG	CD-NE-CZ	8.33	136.06	124.40
1	B	118	ARG	CA-C-N	8.29	131.74	120.54
1	B	118	ARG	C-N-CA	8.29	131.74	120.54
1	E	81	ARG	NE-CZ-NH2	-8.24	111.78	119.20
1	E	94	ASN	CA-CB-CG	8.21	120.81	112.60
1	F	94	ASN	CA-CB-CG	7.92	120.52	112.60
1	F	248	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	F	82	GLY	CA-C-O	-7.79	114.06	122.47
1	E	191	GLY	CA-C-O	7.77	127.27	122.22
1	E	133	ARG	CD-NE-CZ	7.76	135.26	124.40
1	E	205	ARG	NE-CZ-NH1	7.75	129.25	121.50
1	F	170	SER	O-C-N	-7.71	114.23	123.10
1	C	252	ILE	CB-CA-C	7.70	118.11	110.94
1	B	249	GLN	OE1-CD-NE2	-7.67	114.93	122.60
1	D	179	ARG	NE-CZ-NH1	-7.67	113.83	121.50
1	E	176	VAL	N-CA-CB	-7.66	102.40	112.36
1	D	244	THR	O-C-N	-7.63	112.36	122.97
1	H	262	PHE	CA-C-N	7.62	135.15	121.05
1	H	262	PHE	C-N-CA	7.62	135.15	121.05
1	C	94	ASN	CA-CB-CG	7.61	120.21	112.60
1	A	142	PHE	CA-CB-CG	7.60	121.40	113.80
1	A	52	LEU	N-CA-C	-7.59	102.58	112.68
1	F	262	PHE	CA-C-N	7.58	133.30	121.32
1	F	262	PHE	C-N-CA	7.58	133.30	121.32
1	C	252	ILE	CA-C-O	7.52	125.63	119.47
1	C	148	GLY	CA-C-N	7.49	128.29	119.98
1	C	148	GLY	C-N-CA	7.49	128.29	119.98
1	A	126	GLN	CB-CG-CD	7.47	125.29	112.60
1	A	71	ASN	CA-C-O	-7.46	112.51	120.42
1	B	205	ARG	CG-CD-NE	7.44	128.36	112.00
1	D	241	ILE	O-C-N	-7.44	115.08	122.67
1	F	209	ARG	NH1-CZ-NH2	7.42	128.95	119.30
1	H	202	ILE	N-CA-C	7.42	118.18	110.62
1	C	142	PHE	CA-CB-CG	7.41	121.21	113.80
1	A	81	ARG	CG-CD-NE	7.40	128.27	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	66	PHE	CA-CB-CG	7.39	121.19	113.80
1	F	252	ILE	CB-CA-C	7.38	118.86	110.89
1	H	60	VAL	CA-C-O	-7.33	112.33	120.25
1	G	94	ASN	CA-CB-CG	7.31	119.91	112.60
1	G	205	ARG	CB-CG-CD	7.31	128.11	111.30
1	F	244	THR	CA-C-N	-7.26	113.28	123.08
1	F	244	THR	C-N-CA	-7.26	113.28	123.08
1	C	133	ARG	CD-NE-CZ	7.25	134.55	124.40
1	A	219	GLU	CA-C-N	-7.21	113.46	122.84
1	A	219	GLU	C-N-CA	-7.21	113.46	122.84
1	D	209	ARG	O-C-N	-7.15	113.85	122.22
1	F	205	ARG	NE-CZ-NH2	-7.15	112.77	119.20
1	A	66	PHE	CA-CB-CG	7.12	120.92	113.80
1	A	151	LEU	CA-C-O	-7.07	112.99	120.63
1	B	31	GLY	CA-C-O	7.07	126.62	119.27
1	B	81	ARG	NE-CZ-NH2	-7.00	112.90	119.20
1	H	94	ASN	CA-CB-CG	6.99	119.58	112.60
1	C	209	ARG	NH1-CZ-NH2	6.95	128.33	119.30
1	G	187	VAL	CB-CA-C	-6.95	102.16	110.84
1	B	81	ARG	CG-CD-NE	6.93	127.25	112.00
1	C	214	SER	O-C-N	-6.93	114.72	123.24
1	E	142	PHE	CA-CB-CG	6.92	120.72	113.80
1	D	139	ARG	CD-NE-CZ	6.92	134.09	124.40
1	D	176	VAL	N-CA-CB	-6.88	104.15	112.33
1	H	133	ARG	CA-C-O	6.88	127.88	119.97
1	A	86	ILE	N-CA-C	6.86	117.62	110.62
1	G	121	ALA	N-CA-C	6.86	119.63	111.33
1	A	73	ASN	OD1-CG-ND2	-6.84	115.76	122.60
1	B	238	ILE	CA-C-O	6.82	127.83	120.53
1	B	4	GLN	OE1-CD-NE2	-6.82	115.78	122.60
1	D	252	ILE	CB-CA-C	6.80	117.26	110.94
1	E	126	GLN	CB-CG-CD	6.80	124.15	112.60
1	C	60	VAL	N-CA-C	6.79	118.41	111.00
1	D	184	PHE	CA-C-O	6.75	127.91	120.82
1	D	205	ARG	CB-CG-CD	6.73	126.79	111.30
1	H	241	ILE	O-C-N	-6.73	115.45	122.66
1	F	106	GLY	CA-C-O	6.71	126.47	119.02
1	B	237	LYS	CA-C-N	-6.71	114.40	123.12
1	B	237	LYS	C-N-CA	-6.71	114.40	123.12
1	H	52	LEU	N-CA-C	-6.70	103.78	112.68
1	B	200	ASN	OD1-CG-ND2	-6.68	115.92	122.60
1	E	60	VAL	N-CA-C	6.67	120.37	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	178	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	D	10	PHE	CA-C-O	6.64	127.46	120.42
1	H	170	SER	CA-C-O	-6.63	113.53	120.70
1	H	209	ARG	NE-CZ-NH1	-6.63	114.87	121.50
1	A	94	ASN	CA-CB-CG	6.62	119.22	112.60
1	A	175	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	F	121	ALA	N-CA-C	6.61	118.14	111.07
1	C	48	ASP	CA-C-O	-6.59	114.79	122.37
1	C	251	ASN	CA-CB-CG	6.58	119.18	112.60
1	E	248	ASN	CA-CB-CG	6.57	119.17	112.60
1	A	245	GLY	CA-C-O	-6.55	113.86	119.56
1	E	52	LEU	N-CA-C	-6.51	105.34	113.55
1	E	262	PHE	CA-C-N	6.51	133.27	120.84
1	E	262	PHE	C-N-CA	6.51	133.27	120.84
1	A	80	PHE	O-C-N	-6.51	115.92	123.27
1	A	71	ASN	CA-CB-CG	-6.49	106.11	112.60
1	D	119	SER	N-CA-C	6.49	119.19	111.33
1	F	89	TRP	CA-C-O	-6.49	114.01	120.70
1	A	121	ALA	N-CA-C	6.49	119.17	111.71
1	H	195	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	D	162	ASN	CA-CB-CG	-6.40	106.20	112.60
1	C	203	VAL	O-C-N	-6.40	115.53	120.07
1	D	262	PHE	CA-C-N	6.40	131.22	120.86
1	D	262	PHE	C-N-CA	6.40	131.22	120.86
1	D	118	ARG	CA-C-N	6.39	129.14	120.38
1	D	118	ARG	C-N-CA	6.39	129.14	120.38
1	C	203	VAL	CA-C-O	6.36	124.26	118.85
1	H	176	VAL	N-CA-CB	-6.35	104.10	112.36
1	B	133	ARG	NE-CZ-NH1	6.33	127.83	121.50
1	C	139	ARG	NE-CZ-NH2	-6.32	113.51	119.20
1	D	113	PHE	CA-C-N	6.32	128.66	120.44
1	D	113	PHE	C-N-CA	6.32	128.66	120.44
1	D	77	VAL	N-CA-C	6.31	116.95	107.80
1	A	162	ASN	CA-CB-CG	-6.31	106.29	112.60
1	G	10	PHE	CA-CB-CG	6.31	120.11	113.80
1	A	262	PHE	O-C-N	-6.30	114.21	122.59
1	A	80	PHE	CA-C-O	6.29	127.29	120.43
1	D	142	PHE	CA-CB-CG	6.29	120.09	113.80
1	G	126	GLN	CB-CG-CD	6.27	123.26	112.60
1	H	114	THR	CA-C-O	6.24	127.37	120.82
1	E	219	GLU	CA-C-O	-6.24	113.49	120.66
1	F	60	VAL	CA-C-O	-6.24	113.51	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	D	242	ASP	CB-CG-OD2	6.22	132.70	118.40
1	H	244	THR	CA-C-N	-6.19	114.72	123.08
1	H	244	THR	C-N-CA	-6.19	114.72	123.08
1	H	251	ASN	CA-CB-CG	6.19	118.79	112.60
1	D	182	ALA	CA-C-N	6.18	128.56	120.28
1	D	182	ALA	C-N-CA	6.18	128.56	120.28
1	D	193	LEU	CA-C-O	-6.16	113.77	120.36
1	F	60	VAL	N-CA-C	6.13	119.65	111.44
1	A	48	ASP	CA-C-O	-6.11	115.34	122.37
1	B	142	PHE	CA-CB-CG	6.11	119.91	113.80
1	D	244	THR	N-CA-C	-6.11	101.16	110.14
1	F	249	GLN	O-C-N	6.11	126.31	121.55
1	B	32	THR	N-CA-CB	-6.08	101.41	110.17
1	C	64	THR	O-C-N	-6.08	115.85	123.27
1	C	148	GLY	O-C-N	-6.06	116.29	122.17
1	C	214	SER	CA-C-O	6.02	128.15	121.11
1	B	2	VAL	N-CA-CB	6.01	120.94	112.52
1	C	184	PHE	CA-CB-CG	-6.01	107.78	113.80
1	B	239	GLU	CA-C-O	-5.99	114.36	121.66
1	F	144	GLY	CA-C-O	-5.98	115.77	121.87
1	A	179	ARG	N-CA-C	5.97	117.79	111.28
1	D	264	LEU	CA-C-O	-5.97	114.58	121.15
1	A	82	GLY	CA-C-O	-5.96	115.17	122.03
1	C	84	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	H	127	LYS	CA-C-O	-5.95	114.25	120.55
1	F	184	PHE	CA-CB-CG	-5.94	107.86	113.80
1	C	5	ASP	CA-C-O	5.94	127.06	120.82
1	A	152	ALA	CA-C-O	5.93	127.05	120.82
1	H	160	ARG	CA-C-O	-5.93	114.99	121.87
1	H	205	ARG	NE-CZ-NH2	-5.93	113.87	119.20
1	F	52	LEU	N-CA-C	-5.92	104.80	112.68
1	E	254	ASP	N-CA-CB	-5.92	100.51	111.52
1	E	77	VAL	N-CA-C	5.92	116.38	107.80
1	A	165	ASP	CA-CB-CG	-5.90	106.70	112.60
1	G	174	PRO	CA-C-O	-5.90	114.36	122.15
1	F	149	GLY	O-C-N	5.88	128.69	122.28
1	D	89	TRP	CA-C-O	-5.87	114.66	120.82
1	D	102	ASP	O-C-N	-5.87	114.79	122.59
1	A	219	GLU	O-C-N	5.85	130.50	123.36
1	D	121	ALA	N-CA-C	5.85	117.33	111.07
1	F	254	ASP	N-CA-CB	-5.85	100.65	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	HIS	CA-CB-CG	5.83	119.63	113.80
1	C	242	ASP	CB-CG-OD2	5.83	131.81	118.40
1	F	183	GLU	CA-C-O	5.83	126.60	120.42
1	B	68	ALA	N-CA-C	5.83	119.45	110.42
1	G	146	SER	CB-CA-C	-5.82	109.88	116.63
1	B	139	ARG	NE-CZ-NH2	-5.82	113.96	119.20
1	D	133	ARG	CD-NE-CZ	5.82	132.54	124.40
1	A	205	ARG	CB-CG-CD	5.81	124.66	111.30
1	D	252	ILE	N-CA-C	5.79	113.61	108.63
1	C	209	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	B	86	ILE	N-CA-C	5.77	115.96	110.42
1	D	184	PHE	O-C-N	-5.75	116.15	122.07
1	D	205	ARG	CG-CD-NE	5.75	124.65	112.00
1	D	10	PHE	CA-CB-CG	5.73	119.53	113.80
1	B	66	PHE	CA-CB-CG	5.72	119.52	113.80
1	G	244	THR	CA-C-N	-5.71	114.52	122.86
1	G	244	THR	C-N-CA	-5.71	114.52	122.86
1	B	176	VAL	N-CA-CB	-5.71	104.93	112.36
1	F	120	VAL	O-C-N	-5.71	116.60	122.14
1	A	179	ARG	NH1-CZ-NH2	-5.70	111.89	119.30
1	A	195	ARG	CD-NE-CZ	5.70	132.38	124.40
1	B	84	ARG	CD-NE-CZ	5.70	132.38	124.40
1	G	196	ILE	N-CA-C	5.70	116.14	108.17
1	A	237	LYS	CA-C-O	-5.69	114.49	120.58
1	G	175	ARG	N-CA-C	-5.68	103.03	110.53
1	A	203	VAL	N-CA-CB	5.68	114.32	110.52
1	B	60	VAL	N-CA-C	5.67	117.18	111.00
1	H	175	ARG	CD-NE-CZ	5.66	132.33	124.40
1	A	178	ASN	CA-C-O	-5.65	115.59	121.98
1	D	205	ARG	NE-CZ-NH1	5.64	127.14	121.50
1	F	209	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	A	119	SER	CA-C-N	5.64	130.49	122.09
1	A	119	SER	C-N-CA	5.64	130.49	122.09
1	E	238	ILE	CA-C-O	5.64	126.56	120.53
1	A	95	PHE	CA-CB-CG	5.64	119.44	113.80
1	A	77	VAL	CA-C-O	-5.63	114.07	120.66
1	H	95	PHE	CA-CB-CG	5.62	119.42	113.80
1	E	187	VAL	CA-CB-CG1	-5.61	100.86	110.40
1	B	60	VAL	CA-C-O	-5.61	114.71	120.71
1	B	94	ASN	CA-CB-CG	5.60	118.20	112.60
1	D	102	ASP	N-CA-C	-5.59	98.89	110.80
1	F	10	PHE	CA-CB-CG	5.59	119.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	205	ARG	NE-CZ-NH1	5.59	127.09	121.50
1	F	217	SER	CA-C-O	-5.59	113.76	120.41
1	D	15	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	D	146	SER	CA-C-N	5.58	128.31	120.28
1	D	146	SER	C-N-CA	5.58	128.31	120.28
1	A	175	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	G	71	ASN	OD1-CG-ND2	5.56	128.16	122.60
1	G	205	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	D	243	ALA	CA-C-O	5.56	127.99	121.87
1	D	233	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	B	183	GLU	CA-C-O	5.55	126.30	120.42
1	E	132	VAL	N-CA-C	5.54	116.27	110.62
1	D	208	PRO	CA-C-N	5.54	128.25	120.28
1	D	208	PRO	C-N-CA	5.54	128.25	120.28
1	G	149	GLY	N-CA-C	-5.53	107.80	114.66
1	F	70	ASP	CA-CB-CG	5.53	118.13	112.60
1	D	248	ASN	CA-CB-CG	5.53	118.13	112.60
1	A	53	TYR	O-C-N	-5.53	116.48	123.17
1	G	139	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	C	32	THR	N-CA-CB	-5.52	102.47	110.36
1	A	77	VAL	N-CA-C	5.51	115.53	107.37
1	C	241	ILE	O-C-N	-5.51	115.68	122.57
1	H	9	GLN	OE1-CD-NE2	5.50	128.10	122.60
1	E	30	ALA	CA-C-O	-5.50	115.50	121.44
1	A	251	ASN	CA-C-O	-5.49	115.54	121.36
1	D	203	VAL	N-CA-CB	5.49	114.73	110.45
1	D	183	GLU	O-C-N	5.48	127.93	122.12
1	C	262	PHE	CA-C-N	5.48	131.30	120.84
1	C	262	PHE	C-N-CA	5.48	131.30	120.84
1	F	251	ASN	CA-CB-CG	5.46	118.06	112.60
1	D	244	THR	CA-C-N	5.46	130.44	123.08
1	D	244	THR	C-N-CA	5.46	130.44	123.08
1	B	162	ASN	OD1-CG-ND2	5.45	128.05	122.60
1	B	126	GLN	CB-CG-CD	5.45	121.86	112.60
1	A	70	ASP	CA-CB-CG	5.45	118.05	112.60
1	G	241	ILE	O-C-N	-5.44	117.51	122.79
1	H	70	ASP	CA-CB-CG	5.44	118.04	112.60
1	H	60	VAL	N-CA-C	5.43	118.72	111.44
1	G	72	THR	O-C-N	5.43	127.66	122.07
1	F	165	ASP	CA-CB-CG	-5.43	107.17	112.60
1	B	103	ILE	N-CA-C	5.42	115.63	110.53
1	A	60	VAL	N-CA-C	5.41	118.69	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	SER	N-CA-C	5.41	117.34	108.52
1	F	210	GLU	CA-C-O	-5.41	112.29	119.10
1	F	169	PHE	CA-C-O	-5.40	113.76	120.57
1	B	135	HIS	CA-C-N	5.40	125.01	119.56
1	B	135	HIS	C-N-CA	5.40	125.01	119.56
1	G	60	VAL	CA-C-O	-5.40	115.13	120.85
1	C	94	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	H	202	ILE	CA-C-N	5.40	123.64	120.24
1	H	202	ILE	C-N-CA	5.40	123.64	120.24
1	D	193	LEU	CA-C-N	-5.40	115.44	123.11
1	D	193	LEU	C-N-CA	-5.40	115.44	123.11
1	E	84	ARG	CA-CB-CG	5.38	124.87	114.10
1	B	193	LEU	CA-C-O	-5.38	114.57	120.43
1	C	165	ASP	CA-CB-CG	-5.37	107.23	112.60
1	H	195	ARG	CD-NE-CZ	5.37	131.92	124.40
1	B	251	ASN	CA-C-O	-5.37	115.44	121.40
1	A	191	GLY	CA-C-N	5.36	130.54	122.99
1	A	191	GLY	C-N-CA	5.36	130.54	122.99
1	B	251	ASN	CA-CB-CG	5.35	117.95	112.60
1	F	86	ILE	N-CA-C	5.35	116.08	110.62
1	B	245	GLY	CA-C-O	-5.35	113.87	119.27
1	A	251	ASN	CA-CB-CG	5.32	117.92	112.60
1	D	30	ALA	CA-C-O	-5.31	115.92	121.55
1	B	189	THR	CA-C-O	-5.30	115.40	121.82
1	H	151	LEU	CA-C-O	-5.30	115.25	120.82
1	A	168	VAL	O-C-N	-5.30	117.58	123.20
1	A	9	GLN	CA-C-N	5.30	127.39	120.28
1	A	9	GLN	C-N-CA	5.30	127.39	120.28
1	A	73	ASN	CA-CB-CG	5.30	117.90	112.60
1	F	92	ASN	CA-CB-CG	-5.30	107.30	112.60
1	A	132	VAL	N-CA-C	5.29	115.50	110.42
1	D	252	ILE	CA-C-O	5.29	123.81	119.47
1	B	84	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	G	186	THR	CA-C-O	-5.29	114.81	120.42
1	B	33	ASN	CA-CB-CG	5.28	117.88	112.60
1	B	248	ASN	CA-C-O	-5.28	116.03	122.41
1	G	162	ASN	CA-C-N	-5.27	117.71	123.30
1	G	162	ASN	C-N-CA	-5.27	117.71	123.30
1	C	81	ARG	N-CA-CB	-5.27	102.28	110.29
1	C	267	THR	CA-CB-OG1	-5.27	101.70	109.60
1	A	213	TYR	CA-C-O	-5.26	115.21	121.16
1	A	220	TYR	CA-C-O	-5.26	115.07	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	GLU	N-CA-CB	5.25	118.74	110.56
1	F	193	LEU	O-C-N	-5.24	116.81	123.05
1	B	150	ALA	O-C-N	5.24	127.75	122.09
1	E	8	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	D	81	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	D	195	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	D	86	ILE	N-CA-C	5.21	115.83	110.36
1	E	226	THR	CA-C-O	-5.21	114.82	120.81
1	D	52	LEU	N-CA-C	-5.20	104.55	112.04
1	C	133	ARG	CA-C-N	5.20	127.68	120.29
1	C	133	ARG	C-N-CA	5.20	127.68	120.29
1	G	193	LEU	CA-C-O	-5.20	114.60	120.32
1	B	77	VAL	CA-C-O	-5.19	114.59	120.66
1	B	244	THR	CA-C-N	-5.19	116.07	123.08
1	B	244	THR	C-N-CA	-5.19	116.07	123.08
1	C	131	ALA	CA-C-O	-5.19	114.92	120.42
1	F	126	GLN	CB-CG-CD	5.19	121.42	112.60
1	E	121	ALA	N-CA-C	5.17	116.60	111.07
1	H	186	THR	CA-C-O	-5.16	115.08	120.55
1	B	77	VAL	N-CA-C	5.15	115.00	107.37
1	F	242	ASP	CA-C-O	5.14	126.33	119.59
1	G	66	PHE	CA-CB-CG	5.14	118.94	113.80
1	D	132	VAL	N-CA-C	5.13	115.90	110.72
1	C	14	ALA	CA-C-O	5.11	125.97	120.55
1	B	175	ARG	NH1-CZ-NH2	-5.11	112.66	119.30
1	E	120	VAL	CA-C-O	5.11	124.71	119.35
1	D	251	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	B	128	VAL	CA-C-N	5.10	127.12	120.28
1	B	128	VAL	C-N-CA	5.10	127.12	120.28
1	A	84	ARG	CG-CD-NE	5.10	123.22	112.00
1	C	73	ASN	CA-CB-CG	5.09	117.69	112.60
1	H	153	THR	CA-CB-CG2	5.09	119.16	110.50
1	C	32	THR	CA-CB-CG2	5.09	119.15	110.50
1	F	175	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	B	106	GLY	CA-C-O	5.08	124.75	119.06
1	C	119	SER	CB-CA-C	-5.08	102.32	110.74
1	H	12	LEU	CA-C-O	-5.07	115.50	120.82
1	H	115	SER	O-C-N	5.07	127.49	122.12
1	A	9	GLN	CA-C-O	5.07	125.79	120.42
1	B	243	ALA	O-C-N	-5.06	115.86	122.59
1	F	249	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	B	92	ASN	CA-CB-CG	-5.04	107.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	PHE	CA-C-N	5.03	126.98	120.44
1	A	113	PHE	C-N-CA	5.03	126.98	120.44
1	F	17	SER	CA-C-O	5.03	125.89	120.55
1	E	145	HIS	CA-C-O	-5.03	115.27	120.70
1	E	158	ASP	CA-C-O	-5.03	115.52	120.70
1	A	126	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	D	196	ILE	N-CA-C	5.03	115.21	108.17
1	E	241	ILE	O-C-N	-5.03	117.54	122.67
1	A	145	HIS	CA-CB-CG	5.02	118.82	113.80
1	G	228	VAL	O-C-N	5.02	126.18	121.11
1	H	121	ALA	N-CA-C	5.01	116.75	111.28
1	A	224	SER	CB-CA-C	5.01	118.68	109.46
1	F	195	ARG	NE-CZ-NH1	-5.01	116.49	121.50
1	F	208	PRO	CA-C-N	5.01	127.50	120.28
1	F	208	PRO	C-N-CA	5.01	127.50	120.28
1	B	10	PHE	CA-CB-CG	5.01	118.81	113.80
1	G	224	SER	CB-CA-C	5.01	119.94	109.68

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	LEU	Mainchain
1	A	15	GLN	Mainchain
1	A	151	LEU	Mainchain
1	A	168	VAL	Mainchain
1	A	197	THR	Mainchain
1	A	252	ILE	Mainchain
1	A	258	HIS	Mainchain
1	A	45	GLU	Mainchain
1	B	168	VAL	Mainchain
1	B	194	TYR	Mainchain
1	B	261	TYR	Mainchain
1	C	140	VAL	Mainchain
1	C	170	SER	Mainchain
1	C	18	ALA	Mainchain
1	C	193	LEU	Mainchain
1	C	194	TYR	Mainchain
1	C	241	ILE	Mainchain
1	D	102	ASP	Mainchain
1	D	209	ARG	Mainchain
1	D	258	HIS	Mainchain

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Mol	Chain	Res	Type	Group
1	D	262	PHE	Mainchain
1	D	83	SER	Mainchain
1	E	15	GLN	Mainchain
1	E	203	VAL	Mainchain
1	E	253	PRO	Mainchain
1	E	37	THR	Mainchain
1	F	15	GLN	Mainchain
1	F	176	VAL	Mainchain
1	F	245	GLY	Mainchain
1	F	37	THR	Mainchain
1	G	121	ALA	Mainchain
1	G	141	VAL	Mainchain
1	G	168	VAL	Mainchain
1	G	209	ARG	Mainchain
1	G	224	SER	Mainchain
1	G	243	ALA	Mainchain
1	G	252	ILE	Mainchain
1	H	205	ARG	Mainchain
1	H	64	THR	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	2071	0	1965	32	0
1	B	2071	0	1965	31	0
1	C	2071	0	1965	26	0
1	D	2071	0	1965	44	1
1	E	2071	0	1965	35	1
1	F	2071	0	1965	33	0
1	G	2071	0	1965	50	0
1	H	2071	0	1965	39	0
2	A	90	0	0	5	1
2	B	102	0	0	6	1
2	C	64	0	0	4	0
2	D	68	0	0	10	0
2	E	57	0	0	6	0
2	F	51	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	30	0	0	9	0
2	H	51	0	0	6	0
All	All	17081	0	15720	281	2

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 9.

All (281) 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:231:THR:HG21	1:G:125:ARG:HH12	1.21	1.02
1:F:252:ILE:HD12	1:F:253:PRO:HD2	1.50	0.94
1:D:252:ILE:HD12	1:D:253:PRO:HD2	1.52	0.92
1:H:252:ILE:HD12	1:H:253:PRO:HD2	1.51	0.92
1:H:179:ARG:NH2	2:H:270:HOH:O	2.03	0.91
1:F:34:ILE:HB	2:F:300:HOH:O	1.69	0.89
1:C:126:GLN:HG2	2:C:305:HOH:O	1.74	0.86
1:A:48:ASP:HB2	2:A:353:HOH:O	1.77	0.84
1:C:252:ILE:HD12	1:C:253:PRO:HD2	1.58	0.84
1:B:179:ARG:CZ	2:B:284:HOH:O	2.26	0.82
1:A:179:ARG:HD2	1:A:214:SER:OG	1.78	0.82
1:H:179:ARG:CZ	2:H:270:HOH:O	2.28	0.82
1:G:162:ASN:HB3	2:G:292:HOH:O	1.81	0.80
1:C:242:ASP:OD1	2:C:323:HOH:O	2.00	0.78
1:G:34:ILE:HG12	2:G:275:HOH:O	1.82	0.77
1:A:252:ILE:HD12	1:A:253:PRO:HD2	1.66	0.76
1:B:252:ILE:HD12	1:B:253:PRO:HD2	1.67	0.76
1:E:179:ARG:CZ	2:E:282:HOH:O	2.34	0.76
1:B:32:THR:HG21	2:B:334:HOH:O	1.86	0.75
1:G:252:ILE:HD12	1:G:253:PRO:HD2	1.71	0.71
1:C:84:ARG:O	1:C:84:ARG:HD3	1.90	0.71
1:E:179:ARG:HG2	1:E:179:ARG:HH11	1.53	0.71
1:B:29:PRO:O	1:B:32:THR:HB	1.91	0.70
1:G:176:VAL:HG12	2:G:294:HOH:O	1.92	0.69
1:D:84:ARG:O	1:D:84:ARG:HD3	1.91	0.69
1:D:179:ARG:HD2	1:D:214:SER:OG	1.92	0.69
1:A:29:PRO:O	1:A:32:THR:HB	1.93	0.69
1:H:84:ARG:O	1:H:84:ARG:HD3	1.93	0.68
1:C:242:ASP:HA	2:C:323:HOH:O	1.94	0.68
1:D:179:ARG:HH12	1:H:183:GLU:CD	2.02	0.68
1:A:179:ARG:NE	2:A:358:HOH:O	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ARG:HD3	1:D:159:LEU:HD22	1.76	0.67
1:B:84:ARG:O	1:B:84:ARG:HD3	1.95	0.66
1:H:125:ARG:HD3	1:H:159:LEU:HD22	1.76	0.66
1:E:239:GLU:OE2	2:E:297:HOH:O	2.13	0.66
1:F:84:ARG:HD3	1:F:84:ARG:O	1.96	0.65
1:F:179:ARG:HD2	1:F:214:SER:OG	1.97	0.65
1:B:179:ARG:NH2	2:B:284:HOH:O	2.25	0.65
1:H:39:ASN:HA	2:H:294:HOH:O	1.97	0.64
1:B:125:ARG:HD3	1:B:159:LEU:HD22	1.79	0.64
1:D:179:ARG:NE	2:D:324:HOH:O	2.30	0.64
1:A:133:ARG:HG3	1:A:133:ARG:HH11	1.63	0.64
1:A:179:ARG:HD2	1:A:214:SER:HG	1.62	0.64
1:G:139:ARG:HG3	2:G:284:HOH:O	1.97	0.63
1:B:48:ASP:HB2	2:B:332:HOH:O	1.97	0.63
1:B:179:ARG:HG2	1:B:179:ARG:HH11	1.64	0.63
1:C:125:ARG:HD3	1:C:159:LEU:HD22	1.81	0.62
1:G:84:ARG:O	1:G:84:ARG:HD3	2.00	0.62
1:D:30:ALA:HB1	2:D:337:HOH:O	1.99	0.62
1:E:252:ILE:HD12	1:E:253:PRO:HD2	1.81	0.61
1:G:214:SER:OG	1:G:242:ASP:OD2	2.18	0.61
1:A:231:THR:HG21	1:G:125:ARG:NH1	2.05	0.61
1:D:179:ARG:CZ	2:D:270:HOH:O	2.49	0.60
1:G:179:ARG:HD2	1:G:214:SER:OG	2.00	0.60
1:F:81:ARG:HD3	1:F:82:GLY:O	2.01	0.60
1:C:214:SER:OG	1:C:242:ASP:OD2	2.19	0.60
1:D:179:ARG:NH2	2:D:283:HOH:O	2.33	0.59
1:E:241:ILE:O	1:E:242:ASP:HB2	2.01	0.59
1:E:179:ARG:HG2	1:E:179:ARG:NH1	2.17	0.59
1:H:179:ARG:HD2	1:H:214:SER:OG	2.03	0.59
1:E:84:ARG:O	1:E:84:ARG:HD3	2.03	0.59
1:E:179:ARG:HD2	1:E:214:SER:OG	2.03	0.59
1:H:29:PRO:O	1:H:32:THR:HB	2.03	0.59
1:D:179:ARG:CZ	2:D:324:HOH:O	2.51	0.58
1:B:27:ASP:HB2	2:B:344:HOH:O	2.03	0.58
1:G:195:ARG:NH1	1:G:219:GLU:HB2	2.19	0.58
1:C:179:ARG:HD2	1:C:214:SER:OG	2.04	0.57
1:A:179:ARG:CZ	2:A:358:HOH:O	2.51	0.57
1:C:215:HIS:HB2	2:C:323:HOH:O	2.03	0.57
1:G:133:ARG:HH11	1:G:133:ARG:HG3	1.70	0.57
1:D:70:ASP:HB3	1:D:75:LEU:HB2	1.87	0.56
1:F:116:SER:O	1:F:119:SER:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:HD3	1:A:84:ARG:O	2.05	0.56
1:A:1:GLU:HG3	1:A:236:VAL:HG22	1.87	0.56
1:H:33:ASN:HD22	1:H:33:ASN:H	1.53	0.55
1:H:20:ALA:HB1	1:H:81:ARG:HB2	1.87	0.55
1:C:223:LYS:HE2	1:C:236:VAL:HG23	1.89	0.55
1:D:205:ARG:HG2	2:D:298:HOH:O	2.05	0.55
1:E:81:ARG:HD3	1:E:82:GLY:O	2.07	0.54
1:D:214:SER:OG	1:D:242:ASP:OD2	2.21	0.54
1:B:179:ARG:HD2	1:B:214:SER:OG	2.07	0.53
1:C:29:PRO:O	1:C:32:THR:HB	2.08	0.53
1:D:249:GLN:HG2	2:D:308:HOH:O	2.09	0.53
1:G:198:HIS:O	1:G:199:THR:C	2.49	0.53
1:G:34:ILE:CG1	2:G:275:HOH:O	2.49	0.53
1:H:58:SER:HB2	1:H:63:VAL:O	2.07	0.53
1:D:179:ARG:NH1	1:H:183:GLU:CD	2.66	0.53
1:G:29:PRO:O	1:G:32:THR:HB	2.09	0.53
1:B:116:SER:O	1:B:119:SER:HB2	2.08	0.53
1:H:179:ARG:HG2	1:H:179:ARG:HH11	1.74	0.53
1:H:133:ARG:HG3	1:H:133:ARG:HH11	1.74	0.53
1:H:241:ILE:O	1:H:242:ASP:HB2	2.08	0.53
1:D:29:PRO:O	1:D:32:THR:HB	2.09	0.53
1:E:36:CYS:HB3	1:E:40:ALA:HB3	1.91	0.52
1:B:1:GLU:HG3	1:B:236:VAL:HG22	1.91	0.52
1:C:220:TYR:OH	1:C:237:LYS:HE3	2.10	0.52
1:D:81:ARG:HD3	1:D:82:GLY:O	2.10	0.52
1:E:125:ARG:HD3	1:E:159:LEU:HD22	1.91	0.52
1:F:20:ALA:HB1	1:F:81:ARG:HB2	1.91	0.51
1:B:179:ARG:HG2	1:B:179:ARG:NH1	2.22	0.51
1:C:179:ARG:HG2	1:C:179:ARG:HH11	1.75	0.51
1:E:179:ARG:HD2	1:E:214:SER:HG	1.76	0.51
1:F:20:ALA:O	1:F:81:ARG:HG3	2.10	0.51
1:F:95:PHE:CD1	1:F:207:PRO:HB3	2.45	0.51
1:B:53:TYR:CD1	1:B:127:LYS:HE3	2.45	0.51
1:E:232:ARG:HD3	2:E:314:HOH:O	2.09	0.51
1:G:20:ALA:HB1	1:G:81:ARG:HB2	1.93	0.51
1:E:1:GLU:HG3	1:E:236:VAL:HG22	1.92	0.51
1:C:179:ARG:HG2	1:C:179:ARG:NH1	2.24	0.50
1:G:33:ASN:HB3	2:G:281:HOH:O	2.11	0.50
1:G:33:ASN:HD22	1:G:33:ASN:N	2.10	0.50
1:G:206:LEU:HA	1:G:207:PRO:C	2.35	0.50
1:D:179:ARG:NE	2:D:270:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:ARG:NH1	2:F:286:HOH:O	2.44	0.50
1:H:29:PRO:HD3	2:H:312:HOH:O	2.11	0.50
1:E:239:GLU:HG2	2:E:297:HOH:O	2.12	0.50
1:B:220:TYR:OH	1:B:237:LYS:HE3	2.12	0.50
1:F:53:TYR:CD1	1:F:127:LYS:HE3	2.47	0.50
1:G:125:ARG:HD3	1:G:159:LEU:HD22	1.93	0.50
1:A:179:ARG:NH1	2:A:304:HOH:O	2.45	0.49
1:G:254:ASP:CG	1:G:256:PRO:HD2	2.36	0.49
1:H:179:ARG:HG2	1:H:179:ARG:NH1	2.28	0.49
1:B:32:THR:CG2	2:B:334:HOH:O	2.50	0.49
1:A:1:GLU:OE1	1:G:102:ASP:HB3	2.13	0.49
1:A:214:SER:OG	1:A:242:ASP:OD2	2.31	0.49
1:B:128:VAL:O	1:B:132:VAL:HG23	2.12	0.49
1:B:241:ILE:O	1:B:242:ASP:HB2	2.13	0.49
1:H:160:ARG:NH1	2:H:303:HOH:O	2.42	0.49
1:E:29:PRO:O	1:E:32:THR:HB	2.13	0.49
1:H:99:GLU:HG3	2:H:278:HOH:O	2.13	0.48
1:F:70:ASP:CG	1:F:73:ASN:HD22	2.19	0.48
1:D:179:ARG:NH1	1:H:183:GLU:OE2	2.46	0.48
1:D:220:TYR:OH	1:D:237:LYS:HE3	2.13	0.48
1:F:125:ARG:HD3	1:F:159:LEU:HD22	1.96	0.48
1:H:204:PRO:HB2	1:H:247:ASN:OD1	2.13	0.48
1:B:206:LEU:HA	1:B:207:PRO:C	2.38	0.47
1:E:203:VAL:HB	1:E:204:PRO:HD3	1.95	0.47
1:D:264:LEU:CD2	1:G:227:LEU:HD12	2.44	0.47
1:A:81:ARG:HD3	1:A:82:GLY:O	2.15	0.47
1:D:1:GLU:OE2	1:D:233:ASN:O	2.33	0.47
1:G:261:TYR:O	1:G:262:PHE:HB2	2.15	0.47
1:A:254:ASP:CG	1:A:256:PRO:HD2	2.40	0.47
1:G:154:VAL:HG23	1:G:176:VAL:HG21	1.97	0.47
1:C:1:GLU:N	1:C:233:ASN:HA	2.29	0.47
1:E:95:PHE:CD1	1:E:207:PRO:HB3	2.49	0.47
1:H:206:LEU:HA	1:H:207:PRO:C	2.40	0.47
1:F:241:ILE:O	1:F:242:ASP:HB2	2.15	0.47
1:C:260:TRP:HE3	1:C:264:LEU:HD13	1.80	0.46
1:A:53:TYR:CD1	1:A:127:LYS:HE3	2.50	0.46
1:F:128:VAL:O	1:F:132:VAL:HG23	2.15	0.46
1:B:81:ARG:HD3	1:B:82:GLY:O	2.15	0.46
1:G:48:ASP:HB3	2:G:291:HOH:O	2.15	0.46
1:H:49:ALA:HA	1:H:69:LEU:O	2.16	0.46
1:A:247:ASN:OD1	2:A:286:HOH:O	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ARG:NH1	2:G:298:HOH:O	2.49	0.46
1:D:124:LEU:O	1:D:128:VAL:HG23	2.16	0.45
1:G:147:LEU:HD12	1:G:147:LEU:O	2.15	0.45
1:G:179:ARG:O	1:G:183:GLU:HG3	2.16	0.45
1:F:133:ARG:HG3	1:F:133:ARG:HH11	1.82	0.45
1:D:128:VAL:O	1:D:132:VAL:HG23	2.17	0.45
1:G:124:LEU:O	1:G:128:VAL:HG23	2.16	0.45
1:C:53:TYR:CD1	1:C:127:LYS:HE3	2.51	0.45
1:A:58:SER:HB2	1:A:63:VAL:O	2.16	0.45
1:B:1:GLU:N	1:B:233:ASN:HA	2.31	0.45
1:C:58:SER:HB2	1:C:63:VAL:O	2.17	0.45
1:F:58:SER:HB2	1:F:63:VAL:O	2.16	0.45
1:E:206:LEU:HA	1:E:207:PRO:C	2.41	0.45
1:F:29:PRO:O	1:F:32:THR:HB	2.16	0.45
1:A:1:GLU:HA	1:G:102:ASP:HA	1.99	0.45
1:D:1:GLU:HG3	1:D:236:VAL:HG22	1.98	0.45
1:F:207:PRO:HG2	1:F:213:TYR:CE2	2.52	0.45
1:D:179:ARG:NH1	1:H:183:GLU:OE1	2.40	0.45
1:H:261:TYR:O	1:H:262:PHE:HB2	2.16	0.45
1:A:53:TYR:CE1	1:A:127:LYS:HE3	2.52	0.44
1:F:60:VAL:HB	1:F:119:SER:OG	2.17	0.44
1:B:95:PHE:CD1	1:B:207:PRO:HB3	2.52	0.44
1:D:101:ASN:O	1:D:102:ASP:O	2.35	0.44
1:E:53:TYR:CE1	1:E:127:LYS:HE3	2.53	0.44
1:H:179:ARG:HH11	1:H:179:ARG:CG	2.30	0.44
1:D:227:LEU:H	1:D:260:TRP:CG	2.36	0.44
1:E:1:GLU:N	1:E:232:ARG:O	2.50	0.44
1:G:217:SER:OG	1:G:240:GLY:N	2.44	0.44
1:D:179:ARG:CG	1:D:179:ARG:HH11	2.28	0.44
1:D:241:ILE:O	1:D:242:ASP:HB2	2.17	0.44
1:G:220:TYR:OH	1:G:237:LYS:HE3	2.17	0.44
1:H:73:ASN:O	1:H:74:LYS:HB2	2.16	0.44
1:B:195:ARG:NH1	1:B:219:GLU:HB2	2.33	0.44
1:B:198:HIS:O	1:B:199:THR:C	2.59	0.44
1:D:244:THR:HB	2:D:308:HOH:O	2.16	0.44
1:E:269:LEU:HD12	2:E:274:HOH:O	2.18	0.44
1:F:124:LEU:O	1:F:128:VAL:HG23	2.18	0.44
1:G:202:ILE:O	1:G:205:ARG:HB2	2.18	0.44
1:E:53:TYR:CD1	1:E:127:LYS:HE3	2.53	0.43
1:H:33:ASN:HD22	1:H:33:ASN:N	2.11	0.43
1:B:1:GLU:OE2	1:B:233:ASN:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ILE:HD12	2:F:300:HOH:O	2.17	0.43
1:D:179:ARG:NH1	1:D:179:ARG:HG2	2.33	0.43
1:B:179:ARG:HH11	1:B:179:ARG:CG	2.27	0.43
1:C:101:ASN:HA	1:C:104:CYS:O	2.18	0.43
1:E:142:PHE:HZ	1:E:159:LEU:HD12	1.83	0.43
1:D:101:ASN:O	1:D:102:ASP:C	2.56	0.43
1:C:82:GLY:HA2	1:C:148:GLY:H	1.84	0.43
1:E:89:TRP:CD1	2:E:302:HOH:O	2.70	0.43
1:A:1:GLU:HG3	1:A:236:VAL:CG2	2.48	0.43
1:A:206:LEU:HA	1:A:207:PRO:C	2.44	0.43
1:A:227:LEU:H	1:A:260:TRP:CG	2.36	0.43
1:F:70:ASP:OD2	1:F:73:ASN:ND2	2.36	0.43
1:F:206:LEU:HA	1:F:207:PRO:C	2.44	0.43
1:G:33:ASN:H	1:G:33:ASN:ND2	2.17	0.43
1:H:78:LEU:HB3	1:H:142:PHE:CD1	2.54	0.43
1:H:166:ILE:O	1:H:191:GLY:HA3	2.19	0.43
1:A:70:ASP:HB3	1:A:75:LEU:HB2	2.00	0.42
1:C:260:TRP:CE3	1:C:264:LEU:HD13	2.54	0.42
1:D:198:HIS:O	1:D:199:THR:C	2.62	0.42
1:D:252:ILE:HA	1:D:253:PRO:HD3	1.97	0.42
1:D:264:LEU:HD13	1:D:264:LEU:HA	1.90	0.42
1:F:224:SER:CB	2:F:274:HOH:O	2.67	0.42
1:G:28:ALA:HA	1:G:29:PRO:HD3	1.87	0.42
1:G:221:TRP:CZ3	1:G:223:LYS:HG2	2.54	0.42
1:G:227:LEU:HD23	1:G:260:TRP:CZ3	2.53	0.42
1:G:240:GLY:O	1:G:243:ALA:HB2	2.18	0.42
1:A:1:GLU:OE2	1:A:233:ASN:O	2.36	0.42
1:A:133:ARG:HG3	1:A:133:ARG:NH1	2.31	0.42
1:C:98:LYS:HD3	1:C:111:ASP:HA	2.00	0.42
1:H:226:THR:O	1:H:227:LEU:HB2	2.19	0.42
1:E:81:ARG:CD	1:E:82:GLY:O	2.67	0.42
1:F:73:ASN:O	1:F:74:LYS:HB2	2.19	0.42
1:G:33:ASN:HD22	1:G:33:ASN:H	1.66	0.42
1:H:116:SER:O	1:H:119:SER:HB2	2.19	0.42
1:B:133:ARG:HG3	1:B:133:ARG:HH11	1.85	0.42
1:C:226:THR:O	1:C:227:LEU:HB2	2.18	0.42
1:D:1:GLU:HG3	1:D:236:VAL:CG2	2.49	0.42
1:E:1:GLU:H1	1:E:233:ASN:HA	1.84	0.42
1:F:26:ASN:HB3	1:F:56:GLU:HB2	2.02	0.42
1:G:94:ASN:HD21	1:G:96:ASP:HB2	1.85	0.42
1:H:264:LEU:HD13	1:H:264:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ILE:O	1:B:205:ARG:HB2	2.19	0.42
1:G:25:ASN:HA	1:G:51:PHE:CZ	2.54	0.42
1:G:254:ASP:OD1	1:G:256:PRO:HD2	2.20	0.42
1:H:223:LYS:HE2	1:H:236:VAL:HG23	2.01	0.42
1:A:142:PHE:HZ	1:A:159:LEU:HD12	1.85	0.42
1:C:33:ASN:HD22	1:C:33:ASN:H	1.68	0.42
1:H:254:ASP:CG	1:H:256:PRO:HD2	2.44	0.42
1:C:33:ASN:HD22	1:C:33:ASN:N	2.17	0.42
1:D:206:LEU:HA	1:D:207:PRO:C	2.44	0.42
1:E:133:ARG:HG3	1:E:133:ARG:HH11	1.84	0.42
1:A:261:TYR:O	1:A:262:PHE:HB2	2.21	0.41
1:D:81:ARG:CD	1:D:82:GLY:O	2.68	0.41
1:F:179:ARG:NH1	1:F:179:ARG:HG2	2.35	0.41
1:G:164:TYR:HE1	2:G:292:HOH:O	2.03	0.41
1:D:103:ILE:H	1:D:103:ILE:HG13	1.56	0.41
1:F:241:ILE:O	2:F:285:HOH:O	2.22	0.41
1:G:223:LYS:HE3	1:G:223:LYS:HB2	1.77	0.41
1:A:223:LYS:HE3	1:A:223:LYS:HB2	1.91	0.41
1:E:214:SER:OG	1:E:242:ASP:OD2	2.32	0.41
1:G:73:ASN:O	1:G:74:LYS:HB2	2.20	0.41
1:H:198:HIS:O	1:H:199:THR:C	2.63	0.41
1:F:207:PRO:HG2	1:F:213:TYR:CZ	2.56	0.41
1:B:94:ASN:ND2	1:B:96:ASP:OD2	2.54	0.41
1:D:214:SER:HG	1:D:242:ASP:CG	2.22	0.41
1:E:199:THR:OG1	1:E:200:ASN:N	2.48	0.41
1:G:58:SER:HB2	1:G:63:VAL:O	2.20	0.41
1:C:73:ASN:O	1:C:74:LYS:HB2	2.19	0.41
1:D:125:ARG:NE	2:D:319:HOH:O	2.53	0.41
1:E:20:ALA:O	1:E:81:ARG:HG3	2.21	0.41
1:E:142:PHE:O	1:E:168:VAL:HA	2.21	0.41
1:F:201:ASP:O	1:F:204:PRO:HD2	2.20	0.41
1:G:53:TYR:CD1	1:G:127:LYS:HE3	2.56	0.41
1:H:33:ASN:H	1:H:33:ASN:ND2	2.18	0.41
1:D:142:PHE:HZ	1:D:159:LEU:HD12	1.86	0.41
1:E:208:PRO:HG2	1:E:211:PHE:CD1	2.54	0.41
1:F:261:TYR:O	1:F:262:PHE:HB2	2.21	0.41
1:A:86:ILE:HG21	1:A:258:HIS:CD2	2.56	0.41
1:H:1:GLU:HB2	1:H:235:ILE:O	2.21	0.41
1:D:52:LEU:HD13	1:D:131:ALA:HB2	2.03	0.40
1:E:89:TRP:CZ2	1:E:147:LEU:HB2	2.56	0.40
1:F:53:TYR:CE1	1:F:127:LYS:HE3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:PHE:HZ	1:B:159:LEU:HD12	1.86	0.40
1:E:15:GLN:OE1	1:E:43:GLU:HB2	2.21	0.40
1:G:52:LEU:HB2	1:G:67:LEU:O	2.21	0.40
1:G:186:THR:HG23	1:G:217:SER:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:311:HOH:O	2:B:361:HOH:O[2_546]	1.97	0.23
1:D:102:ASP:O	1:E:232:ARG:NH2[2_657]	2.13	0.07

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	267/269 (99%)	256 (96%)	10 (4%)	1 (0%)	30	43
1	B	267/269 (99%)	257 (96%)	9 (3%)	1 (0%)	30	43
1	C	267/269 (99%)	255 (96%)	11 (4%)	1 (0%)	30	43
1	D	267/269 (99%)	256 (96%)	8 (3%)	3 (1%)	11	18
1	E	267/269 (99%)	254 (95%)	12 (4%)	1 (0%)	30	43
1	F	267/269 (99%)	256 (96%)	10 (4%)	1 (0%)	30	43
1	G	267/269 (99%)	256 (96%)	10 (4%)	1 (0%)	30	43
1	H	267/269 (99%)	257 (96%)	9 (3%)	1 (0%)	30	43
All	All	2136/2152 (99%)	2047 (96%)	79 (4%)	10 (0%)	24	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	102	ASP
1	A	199	THR
1	E	199	THR
1	H	199	THR
1	C	199	THR
1	D	199	THR
1	F	199	THR
1	G	199	THR
1	B	199	THR
1	D	103	ILE

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	220/220 (100%)	201 (91%)	19 (9%)	10	16
1	B	220/220 (100%)	200 (91%)	20 (9%)	9	14
1	C	220/220 (100%)	200 (91%)	20 (9%)	9	14
1	D	220/220 (100%)	197 (90%)	23 (10%)	6	10
1	E	220/220 (100%)	198 (90%)	22 (10%)	7	11
1	F	220/220 (100%)	200 (91%)	20 (9%)	9	14
1	G	220/220 (100%)	202 (92%)	18 (8%)	10	18
1	H	220/220 (100%)	203 (92%)	17 (8%)	12	20
All	All	1760/1760 (100%)	1601 (91%)	159 (9%)	9	15

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	32	THR
1	A	33	ASN
1	A	54	SER
1	A	58	SER
1	A	81	ARG

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Mol	Chain	Res	Type
1	A	94	ASN
1	A	102	ASP
1	A	118	ARG
1	A	119	SER
1	A	133	ARG
1	A	146	SER
1	A	162	ASN
1	A	179	ARG
1	A	205	ARG
1	A	214	SER
1	A	252	ILE
1	A	264	LEU
1	A	269	LEU
1	B	1	GLU
1	B	32	THR
1	B	33	ASN
1	B	54	SER
1	B	58	SER
1	B	81	ARG
1	B	84	ARG
1	B	94	ASN
1	B	102	ASP
1	B	118	ARG
1	B	119	SER
1	B	133	ARG
1	B	162	ASN
1	B	176	VAL
1	B	179	ARG
1	B	205	ARG
1	B	239	GLU
1	B	252	ILE
1	B	264	LEU
1	B	269	LEU
1	C	1	GLU
1	C	24	LYS
1	C	33	ASN
1	C	54	SER
1	C	58	SER
1	C	81	ARG
1	C	84	ARG
1	C	94	ASN
1	C	102	ASP

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Mol	Chain	Res	Type
1	C	118	ARG
1	C	119	SER
1	C	133	ARG
1	C	146	SER
1	C	162	ASN
1	C	179	ARG
1	C	205	ARG
1	C	214	SER
1	C	252	ILE
1	C	264	LEU
1	C	269	LEU
1	D	1	GLU
1	D	24	LYS
1	D	33	ASN
1	D	54	SER
1	D	58	SER
1	D	81	ARG
1	D	94	ASN
1	D	98	LYS
1	D	102	ASP
1	D	118	ARG
1	D	119	SER
1	D	129	GLU
1	D	133	ARG
1	D	146	SER
1	D	162	ASN
1	D	176	VAL
1	D	179	ARG
1	D	205	ARG
1	D	214	SER
1	D	250	PRO
1	D	252	ILE
1	D	264	LEU
1	D	269	LEU
1	E	1	GLU
1	E	24	LYS
1	E	33	ASN
1	E	54	SER
1	E	58	SER
1	E	81	ARG
1	E	84	ARG
1	E	94	ASN

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Mol	Chain	Res	Type
1	E	102	ASP
1	E	118	ARG
1	E	119	SER
1	E	133	ARG
1	E	146	SER
1	E	162	ASN
1	E	176	VAL
1	E	179	ARG
1	E	205	ARG
1	E	214	SER
1	E	215	HIS
1	E	252	ILE
1	E	264	LEU
1	E	269	LEU
1	F	1	GLU
1	F	33	ASN
1	F	54	SER
1	F	58	SER
1	F	60	VAL
1	F	81	ARG
1	F	94	ASN
1	F	102	ASP
1	F	118	ARG
1	F	119	SER
1	F	133	ARG
1	F	146	SER
1	F	162	ASN
1	F	176	VAL
1	F	179	ARG
1	F	205	ARG
1	F	214	SER
1	F	252	ILE
1	F	264	LEU
1	F	269	LEU
1	G	1	GLU
1	G	24	LYS
1	G	33	ASN
1	G	54	SER
1	G	58	SER
1	G	94	ASN
1	G	102	ASP
1	G	118	ARG

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Mol	Chain	Res	Type
1	G	119	SER
1	G	133	ARG
1	G	146	SER
1	G	162	ASN
1	G	205	ARG
1	G	214	SER
1	G	215	HIS
1	G	252	ILE
1	G	264	LEU
1	G	269	LEU
1	H	1	GLU
1	H	33	ASN
1	H	58	SER
1	H	84	ARG
1	H	94	ASN
1	H	102	ASP
1	H	118	ARG
1	H	119	SER
1	H	133	ARG
1	H	146	SER
1	H	162	ASN
1	H	176	VAL
1	H	179	ARG
1	H	205	ARG
1	H	252	ILE
1	H	264	LEU
1	H	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	88	ASN
1	A	126	GLN
1	B	11	ASN
1	B	126	GLN
1	C	11	ASN
1	C	33	ASN
1	D	11	ASN
1	D	33	ASN
1	E	33	ASN
1	E	88	ASN

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Mol	Chain	Res	Type
1	E	126	GLN
1	F	11	ASN
1	F	33	ASN
1	F	71	ASN
1	G	11	ASN
1	G	33	ASN
1	G	88	ASN
1	G	126	GLN
1	H	11	ASN
1	H	33	ASN
1	H	126	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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.