Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:04 PM GMT

PDB ID	:	1DT5
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

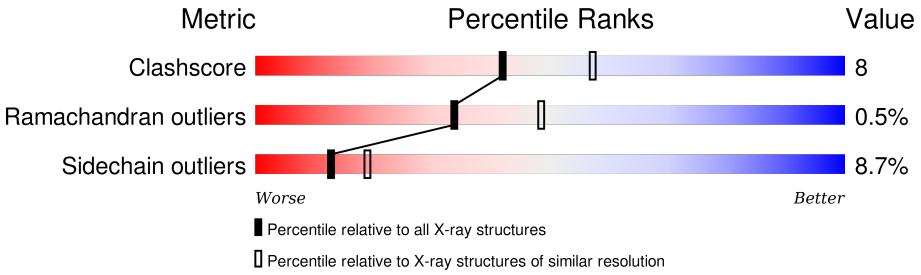
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	269	77% 17% 5% •
1	B	269	76% 17% 6% •
1	C	269	76% 20% • •
1	D	269	77% 17% 5% •
1	E	269	76% 19% • •
1	F	269	75% 20% • •
1	G	269	71% 22% 6% •

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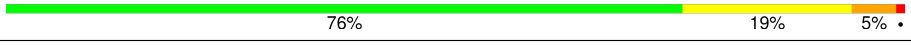
Mol	Chain	Length	Quality of chain
1	H	269	

2 Entry composition (i)

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 O 30 30	0	0
2	H	51	Total O 51 51	0	0

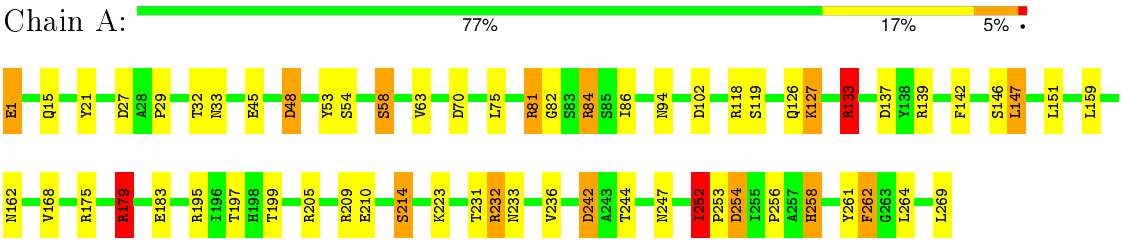
3 Residue-property plots (i)

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

Note EDS was not executed.

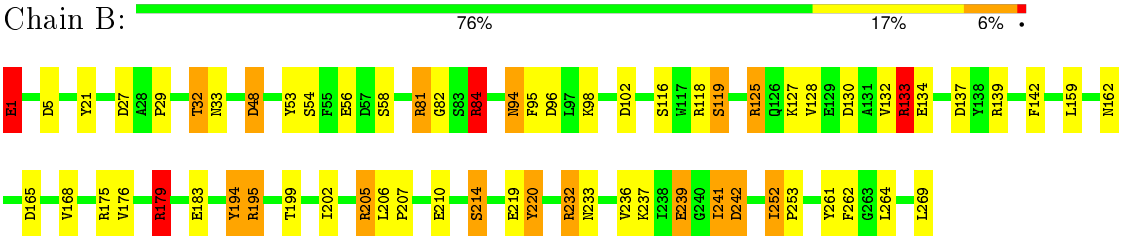
- Molecule 1: LIPASE

Chain A:



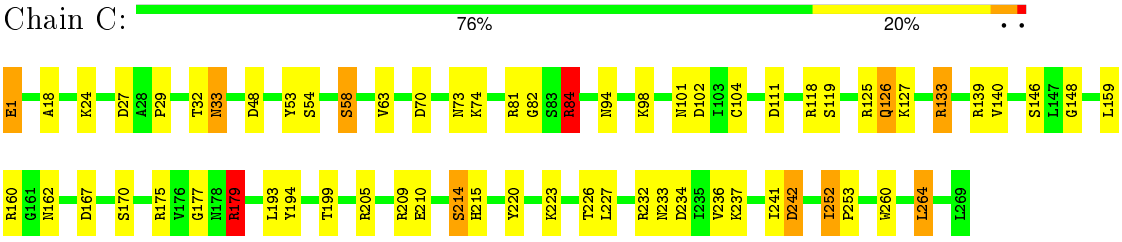
- Molecule 1: LIPASE

Chain B:



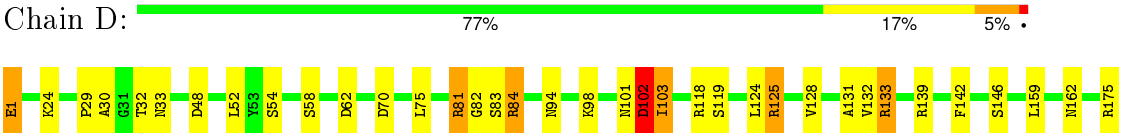
- Molecule 1: LIPASE

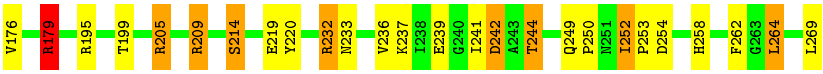
Chain C:



- Molecule 1: LIPASE

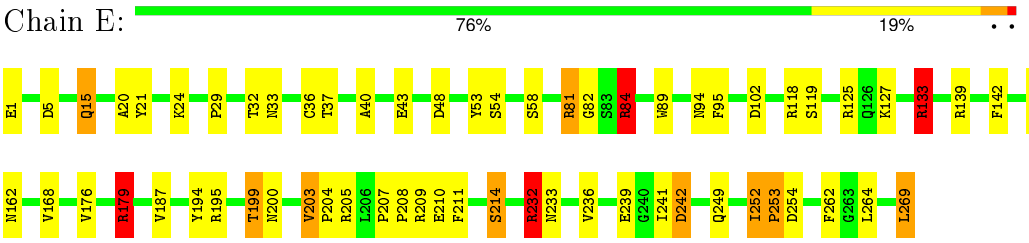
Chain D:





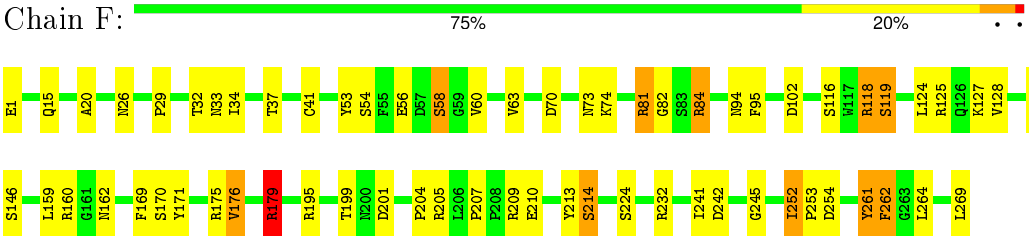
• Molecule 1: LIPASE

Chain E:



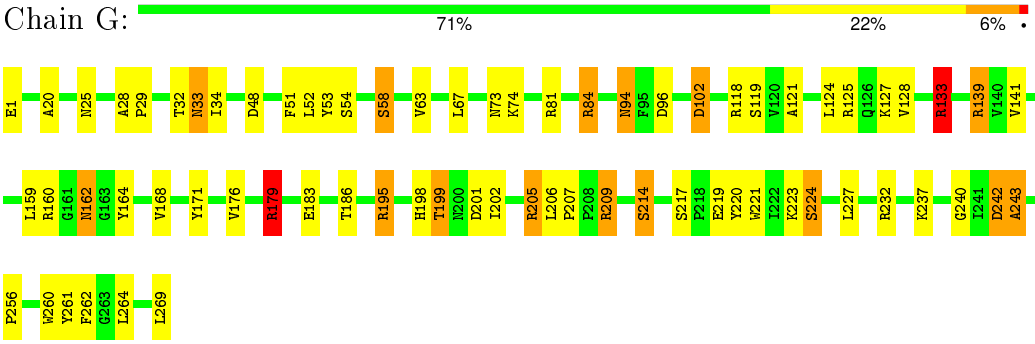
• Molecule 1: LIPASE

Chain F:



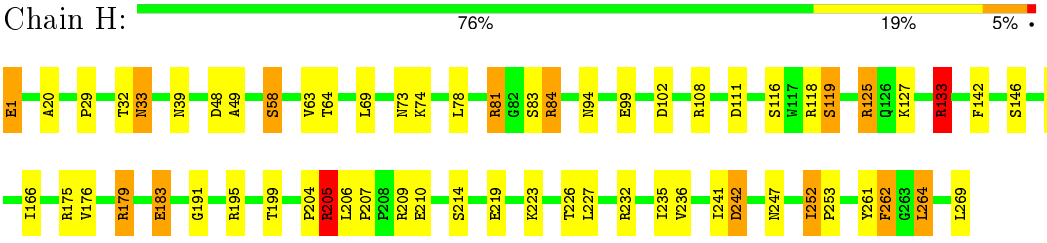
• Molecule 1: LIPASE

Chain G:



• Molecule 1: LIPASE

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.67	0/2121	1.67	38/2887 (1.3%)
1	B	0.69	1/2121 (0.0%)	1.74	39/2887 (1.4%)
1	C	0.57	0/2121	1.54	27/2887 (0.9%)
1	D	0.60	0/2121	1.59	30/2887 (1.0%)
1	E	0.54	0/2121	1.55	32/2887 (1.1%)
1	F	0.56	0/2121	1.55	29/2887 (1.0%)
1	G	0.52	0/2121	1.42	20/2887 (0.7%)
1	H	0.55	0/2121	1.52	21/2887 (0.7%)
All	All	0.59	1/16968 (0.0%)	1.58	236/23096 (1.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	ARG	CD-NE	-5.61	1.36	1.46

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	205	ARG	CD-NE-CZ	25.18	158.84	123.60
1	H	205	ARG	CD-NE-CZ	24.04	157.25	123.60
1	F	205	ARG	NE-CZ-NH1	21.41	131.00	120.30
1	D	205	ARG	CD-NE-CZ	21.20	153.28	123.60
1	E	205	ARG	NE-CZ-NH2	-20.43	110.08	120.30
1	A	205	ARG	CD-NE-CZ	20.30	152.03	123.60
1	A	81	ARG	NE-CZ-NH1	20.15	130.37	120.30
1	A	205	ARG	NE-CZ-NH1	19.52	130.06	120.30
1	E	205	ARG	NE-CZ-NH1	17.91	129.25	120.30
1	B	175	ARG	NE-CZ-NH2	17.82	129.21	120.30
1	E	81	ARG	NE-CZ-NH2	-17.04	111.78	120.30
1	A	179	ARG	NE-CZ-NH2	16.89	128.75	120.30
1	D	242	ASP	CB-CG-OD2	16.00	132.70	118.30
1	F	205	ARG	NE-CZ-NH2	-15.06	112.77	120.30
1	B	133	ARG	NE-CZ-NH1	15.05	127.83	120.30
1	C	242	ASP	CB-CG-OD2	15.01	131.81	118.30
1	B	81	ARG	NE-CZ-NH2	-14.80	112.90	120.30
1	C	205	ARG	CD-NE-CZ	14.62	144.07	123.60
1	C	84	ARG	NE-CZ-NH1	14.31	127.46	120.30
1	G	205	ARG	CD-NE-CZ	13.77	142.87	123.60
1	F	205	ARG	CD-NE-CZ	13.70	142.77	123.60
1	D	205	ARG	NE-CZ-NH1	13.69	127.14	120.30
1	H	205	ARG	NE-CZ-NH1	13.59	127.09	120.30
1	C	139	ARG	NE-CZ-NH2	-13.58	113.51	120.30
1	G	205	ARG	NE-CZ-NH1	13.53	127.06	120.30
1	D	179	ARG	NE-CZ-NH1	-12.93	113.83	120.30
1	H	205	ARG	NE-CZ-NH2	-12.87	113.87	120.30
1	B	139	ARG	NE-CZ-NH2	-12.67	113.96	120.30
1	E	205	ARG	CD-NE-CZ	12.29	140.81	123.60
1	G	139	ARG	NE-CZ-NH2	-12.14	114.23	120.30
1	H	242	ASP	CB-CG-OD2	12.04	129.14	118.30
1	B	84	ARG	NE-CZ-NH2	-11.73	114.44	120.30
1	D	81	ARG	NE-CZ-NH2	-11.61	114.50	120.30
1	C	179	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	H	133	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	H	209	ARG	NE-CZ-NH1	-10.87	114.87	120.30
1	C	205	ARG	NE-CZ-NH2	-10.84	114.88	120.30
1	D	125	ARG	NE-CZ-NH2	-10.75	114.92	120.30
1	A	81	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	G	179	ARG	NE-CZ-NH2	-10.49	115.06	120.30
1	G	84	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	F	209	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	D	205	ARG	NE-CZ-NH2	-10.34	115.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	133	ARG	NE-CZ-NH1	10.33	125.46	120.30
1	B	165	ASP	CB-CG-OD2	-10.29	109.04	118.30
1	E	195	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	A	242	ASP	CB-CG-OD2	10.20	127.48	118.30
1	B	84	ARG	NE-CZ-NH1	10.11	125.35	120.30
1	G	209	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	H	210	GLU	OE1-CD-OE2	-9.95	111.36	123.30
1	A	175	ARG	NE-CZ-NH2	9.70	125.15	120.30
1	B	133	ARG	CD-NE-CZ	9.63	137.09	123.60
1	H	195	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	F	118	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	E	139	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	E	179	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	E	232	ARG	CD-NE-CZ	9.28	136.59	123.60
1	G	133	ARG	CD-NE-CZ	9.19	136.47	123.60
1	A	205	ARG	CG-CD-NE	9.18	131.07	111.80
1	C	209	ARG	NE-CZ-NH1	-9.16	115.72	120.30
1	A	133	ARG	CD-NE-CZ	9.05	136.28	123.60
1	F	133	ARG	CD-NE-CZ	9.04	136.25	123.60
1	H	133	ARG	CD-NE-CZ	8.90	136.06	123.60
1	F	209	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	E	254	ASP	CB-CG-OD1	-8.85	110.33	118.30
1	D	81	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	B	134	GLU	OE1-CD-OE2	-8.78	112.77	123.30
1	A	175	ARG	NE-CZ-NH1	-8.73	115.93	120.30
1	H	242	ASP	CB-CG-OD1	-8.73	110.44	118.30
1	C	209	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	A	133	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	F	209	ARG	NH1-CZ-NH2	8.68	128.95	119.40
1	A	205	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	G	139	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	H	81	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	E	133	ARG	CD-NE-CZ	8.33	135.26	123.60
1	E	242	ASP	CB-CG-OD2	8.31	125.78	118.30
1	A	232	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	D	62	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	B	205	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	G	242	ASP	CB-CG-OD2	8.17	125.65	118.30
1	B	220	TYR	CB-CG-CD1	8.16	125.89	121.00
1	E	81	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	C	209	ARG	NH1-CZ-NH2	8.12	128.33	119.40
1	D	84	ARG	NE-CZ-NH2	-8.10	116.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	195	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	A	137	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	B	205	ARG	CG-CD-NE	7.89	128.36	111.80
1	D	219	GLU	OE1-CD-OE2	-7.88	113.85	123.30
1	A	81	ARG	CG-CD-NE	7.84	128.27	111.80
1	C	133	ARG	CD-NE-CZ	7.82	134.55	123.60
1	F	195	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	F	84	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	H	125	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	F	254	ASP	CB-CG-OD1	-7.55	111.51	118.30
1	B	242	ASP	CB-CG-OD2	7.50	125.05	118.30
1	D	139	ARG	CD-NE-CZ	7.49	134.09	123.60
1	H	108	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	81	ARG	CG-CD-NE	7.36	127.25	111.80
1	C	205	ARG	CB-CG-CD	7.33	130.66	111.60
1	A	48	ASP	CB-CG-OD1	7.22	124.80	118.30
1	B	183	GLU	OE1-CD-OE2	-7.20	114.66	123.30
1	F	84	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	F	179	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	F	179	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	F	133	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	G	242	ASP	CB-CG-OD1	-7.08	111.93	118.30
1	H	175	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	B	48	ASP	CA-CB-CG	7.04	128.89	113.40
1	D	239	GLU	OE1-CD-OE2	6.96	131.65	123.30
1	F	175	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	A	48	ASP	CA-CB-CG	6.92	128.63	113.40
1	B	5	ASP	CB-CG-OD2	6.90	124.51	118.30
1	G	160	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	179	ARG	NH1-CZ-NH2	-6.83	111.89	119.40
1	D	254	ASP	CB-CG-OD2	6.78	124.40	118.30
1	B	125	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	C	160	ARG	NE-CZ-NH2	6.71	123.65	120.30
1	D	209	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	E	187	VAL	CA-CB-CG1	-6.69	100.86	110.90
1	F	210	GLU	OE1-CD-OE2	-6.69	115.27	123.30
1	G	171	TYR	CB-CG-CD1	-6.67	117.00	121.00
1	B	48	ASP	CB-CG-OD1	6.66	124.29	118.30
1	B	210	GLU	OE1-CD-OE2	-6.58	115.40	123.30
1	B	262	PHE	C-N-CA	6.58	136.12	122.30
1	B	195	ARG	NE-CZ-NH1	-6.57	117.01	120.30
1	E	194	TYR	CB-CG-CD2	-6.54	117.08	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	84	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	C	126	GLN	CB-CG-CD	6.50	128.49	111.60
1	E	232	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	B	130	ASP	CB-CG-OD1	6.42	124.08	118.30
1	B	239	GLU	OE1-CD-OE2	6.42	131.00	123.30
1	D	242	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	D	133	ARG	CD-NE-CZ	6.39	132.54	123.60
1	D	244	THR	O-C-N	-6.37	112.36	123.20
1	G	205	ARG	CB-CG-CD	6.35	128.11	111.60
1	A	209	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	B	1	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	B	133	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	195	ARG	CD-NE-CZ	6.27	132.38	123.60
1	B	84	ARG	CD-NE-CZ	6.27	132.38	123.60
1	H	175	ARG	CD-NE-CZ	6.23	132.33	123.60
1	C	48	ASP	CB-CG-OD1	6.19	123.87	118.30
1	D	254	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	B	21	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	E	133	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	175	ARG	NH1-CZ-NH2	-6.13	112.66	119.40
1	H	262	PHE	C-N-CA	6.12	135.15	122.30
1	D	205	ARG	CG-CD-NE	6.12	124.65	111.80
1	F	169	PHE	CB-CG-CD1	6.11	125.08	120.80
1	C	133	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	B	232	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	210	GLU	OE1-CD-OE2	-6.04	116.05	123.30
1	A	244	THR	C-N-CA	-6.01	109.68	122.30
1	C	167	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	70	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	C	81	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	H	195	ARG	CD-NE-CZ	5.94	131.92	123.60
1	D	232	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	C	48	ASP	CA-CB-CG	5.85	126.28	113.40
1	D	205	ARG	CB-CG-CD	5.84	126.79	111.60
1	D	62	ASP	CB-CG-OD1	5.83	123.55	118.30
1	E	210	GLU	OE1-CD-OE2	-5.79	116.36	123.30
1	E	249	GLN	OE1-CD-NE2	-5.78	108.62	121.90
1	G	171	TYR	CB-CG-CD2	5.78	124.47	121.00
1	E	187	VAL	CG1-CB-CG2	5.75	120.11	110.90
1	A	21	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	A	183	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	E	195	ARG	NH1-CZ-NH2	-5.70	113.13	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	160	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	F	175	ARG	NH1-CZ-NH2	-5.68	113.15	119.40
1	E	209	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	H	219	GLU	OE1-CD-OE2	-5.66	116.50	123.30
1	C	210	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	F	171	TYR	CB-CG-CD1	-5.65	117.61	121.00
1	F	261	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	E	21	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	E	48	ASP	CA-CB-CG	5.63	125.79	113.40
1	A	209	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	E	254	ASP	OD1-CG-OD2	5.61	133.95	123.30
1	E	254	ASP	N-CA-CB	-5.61	100.51	110.60
1	A	262	PHE	C-N-CA	5.61	134.07	122.30
1	B	179	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	E	249	GLN	CG-CD-NE2	5.60	130.14	116.70
1	B	241	ILE	O-C-N	-5.59	113.76	122.70
1	A	242	ASP	CB-CG-OD1	-5.55	113.30	118.30
1	F	175	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	195	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	D	209	ARG	O-C-N	-5.53	113.85	122.70
1	F	254	ASP	N-CA-CB	-5.53	100.65	110.60
1	B	194	TYR	CB-CG-CD1	-5.51	117.70	121.00
1	C	205	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	H	111	ASP	CB-CG-OD1	5.46	123.21	118.30
1	D	175	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	B	139	ARG	CD-NE-CZ	5.45	131.23	123.60
1	C	27	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	84	ARG	CG-CD-NE	5.44	123.22	111.80
1	G	209	ARG	NH1-CZ-NH2	5.43	125.37	119.40
1	A	209	ARG	NH1-CZ-NH2	5.39	125.32	119.40
1	A	133	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	G	133	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	56	GLU	OE1-CD-OE2	5.33	129.69	123.30
1	E	242	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	27	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	147	LEU	CB-CG-CD1	5.31	120.03	111.00
1	B	81	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	D	232	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	48	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	177	GLY	CA-C-O	5.30	130.14	120.60
1	F	41	CYS	CA-CB-SG	5.29	123.53	114.00
1	F	170	SER	O-C-N	-5.29	114.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	PHE	O-C-N	-5.29	114.21	123.20
1	H	183	GLU	OE1-CD-OE2	-5.29	116.96	123.30
1	A	126	GLN	CB-CG-CD	5.27	125.29	111.60
1	A	254	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	D	81	ARG	CG-CD-NE	5.27	122.86	111.80
1	C	234	ASP	CB-CG-OD2	5.25	123.03	118.30
1	C	242	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	E	5	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	G	254	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	E	48	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	139	ARG	CD-NE-CZ	5.24	130.94	123.60
1	F	262	PHE	C-N-CA	5.24	133.30	122.30
1	H	48	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	B	239	GLU	CG-CD-OE2	-5.24	107.83	118.30
1	E	262	PHE	C-N-CA	5.22	133.27	122.30
1	C	175	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	E	84	ARG	CA-CB-CG	5.21	124.87	113.40
1	G	224	SER	CB-CA-C	5.18	119.94	110.10
1	B	137	ASP	CB-CG-OD1	5.14	122.92	118.30
1	E	21	TYR	CB-CG-CD1	5.13	124.08	121.00
1	G	201	ASP	CB-CG-OD2	5.07	122.86	118.30
1	F	254	ASP	OD1-CG-OD2	5.06	132.91	123.30
1	G	195	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	F	139	ARG	CD-NE-CZ	5.04	130.66	123.60
1	A	205	ARG	CB-CG-CD	5.03	124.66	111.60

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

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Mol	Chain	Res	Type	Group
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
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2071	0	1965	30	0
1	B	2071	0	1965	31	0
1	C	2071	0	1965	26	0
1	D	2071	0	1965	41	1
1	E	2071	0	1965	33	1
1	F	2071	0	1965	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2071	0	1965	50	0
1	H	2071	0	1965	37	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	5	0
2	F	51	0	0	5	0
2	G	30	0	0	9	0
2	H	51	0	0	6	0
All	All	17081	0	15720	271	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 8.

All (271) 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:E:179:ARG:CZ	2:E:282:HOH:O	2.34	0.76
1:B:252:ILE:HD12	1:B:253:PRO:HD2	1.67	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:HH11	1:E:179:ARG:HG2	1.53	0.71
1:B:29:PRO:O	1:B:32:THR:HB	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:VAL:HG12	2:G:294:HOH:O	1.92	0.69
1:D:179:ARG:HD2	1:D:214:SER:OG	1.92	0.69
1:D:84:ARG:HD3	1:D:84:ARG:O	1.91	0.69
1:A:29:PRO:O	1:A:32:THR:HB	1.93	0.69
1:H:84:ARG:HD3	1:H:84:ARG:O	1.93	0.68
1:C:242:ASP:HA	2:C:323:HOH:O	1.94	0.68
1:A:179:ARG:NE	2:A:358:HOH:O	2.26	0.67
1:D:125:ARG:HD3	1:D:159:LEU:HD22	1.76	0.67
1:B:84:ARG:HD3	1:B:84:ARG:O	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:D:179:ARG:NE	2:D:324:HOH:O	2.30	0.64
1:B:125:ARG:HD3	1:B:159:LEU:HD22	1.79	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:D:179:ARG:HH12	1:H:183:GLU:CD	2.02	0.63
1:B:48:ASP:HB2	2:B:332:HOH:O	1.97	0.63
1:B:179:ARG:HH11	1:B:179:ARG:HG2	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:E:241:ILE:O	1:E:242:ASP:HB2	2.01	0.60
1:D:179:ARG:NH2	2:D:283:HOH:O	2.33	0.59
1:D:214:SER:OG	1:D:242:ASP:OD2	2.21	0.59
1:E:179:ARG:NH1	1:E:179:ARG:HG2	2.17	0.59
1:H:179:ARG:HD2	1:H:214:SER:OG	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:E:84:ARG:O	1:E:84:ARG:HD3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:G:133:ARG:HH11	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
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:B:179:ARG:HD2	1:B:214:SER:OG	2.07	0.53
1:D:249:GLN:HG2	2:D:308:HOH:O	2.09	0.53
1:C:29:PRO:O	1:C:32:THR:HB	2.08	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: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:HH11	1:H:179:ARG:HG2	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:HH11	1:C:179:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:179:ARG:NE	2:D:270:HOH:O	2.44	0.50
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:G:125:ARG:HD3	1:G:159:LEU:HD22	1.93	0.50
1:F:53:TYR:CD1	1:F:127:LYS:HE3	2.47	0.50
1:B:220:TYR:OH	1:B:237:LYS:HE3	2.12	0.50
1:A:179:ARG:NH1	2:A:304:HOH:O	2.45	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:214:SER:OG	1:A:242:ASP:OD2	2.31	0.49
1:A:1:GLU:OE1	1:G:102:ASP:HB3	2.13	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:G:198:HIS:O	1:G:199:THR:C	2.49	0.49
1:D:179:ARG:NH1	1:H:183:GLU:CD	2.66	0.48
1:H:99:GLU:HG3	2:H:278:HOH:O	2.13	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: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:D:1:GLU:OE2	1:D:233:ASN:O	2.33	0.47
1:A:81:ARG:HD3	1:A:82:GLY:O	2.15	0.47
1:G:261:TYR:O	1:G:262:PHE:HB2	2.15	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:F:241:ILE:O	1:F:242:ASP:HB2	2.15	0.47
1:B:179:ARG:HD2	1:B:214:SER:HG	1.80	0.46
1:C:260:TRP:HE3	1:C:264:LEU:HD13	1.80	0.46
1:G:206:LEU:HA	1:G:207:PRO:C	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:73:ASN:O	1:H:74:LYS:HB2	2.16	0.46
1:G:125:ARG:NH1	2:G:298:HOH:O	2.49	0.46
1:A:247:ASN:OD1	2:A:286:HOH:O	2.20	0.46
1:D:124:LEU:O	1:D:128:VAL:HG23	2.16	0.45
1:G:179:ARG:O	1:G:183:GLU:HG3	2.16	0.45
1:G:147:LEU:O	1:G:147:LEU:HD12	2.15	0.45
1:F:133:ARG:HH11	1:F:133:ARG:HG3	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:G:254:ASP:CG	1:G:256:PRO:HD2	2.36	0.45
1:B:1:GLU:N	1:B:233:ASN:HA	2.31	0.45
1:A:58:SER:HB2	1:A:63:VAL:O	2.16	0.45
1:F:58:SER:HB2	1:F:63:VAL:O	2.16	0.45
1:C:58:SER:HB2	1:C:63:VAL:O	2.17	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:F:207:PRO:HG2	1:F:213:TYR:CE2	2.52	0.45
1:D:1:GLU:HG3	1:D:236:VAL:HG22	1.98	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:F:60:VAL:HB	1:F:119:SER:OG	2.17	0.44
1:A:53:TYR:CE1	1:A:127:LYS:HE3	2.52	0.44
1:B:95:PHE:CD1	1:B:207:PRO:HB3	2.52	0.44
1:H:179:ARG:HH11	1:H:179:ARG:CG	2.30	0.44
1:E:53:TYR:CE1	1:E:127:LYS:HE3	2.53	0.44
1:D:101:ASN:O	1:D:102:ASP:O	2.35	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:D:244:THR:HB	2:D:308:HOH:O	2.16	0.44
1:F:124:LEU:O	1:F:128:VAL:HG23	2.18	0.44
1:D:101:ASN:O	1:D:102:ASP:C	2.56	0.44
1:B:195:ARG:NH1	1:B:219:GLU:HB2	2.33	0.44
1:G:202:ILE:O	1:G:205:ARG:HB2	2.18	0.44
1:E:269:LEU:HD12	2:E:274:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:ASN:N	1:H:33:ASN:HD22	2.11	0.43
1:E:53:TYR:CD1	1:E:127:LYS:HE3	2.53	0.43
1:F:70:ASP:CG	1:F:73:ASN:HD22	2.19	0.43
1:F:34:ILE:HD12	2:F:300:HOH:O	2.17	0.43
1:B:1:GLU:OE2	1:B:233:ASN:O	2.36	0.43
1:D:179:ARG:NH1	1:D:179:ARG:HG2	2.33	0.43
1:C:226:THR:O	1:C:227:LEU:HB2	2.18	0.43
1:B:179:ARG:HH11	1:B:179:ARG:CG	2.27	0.43
1:E:142:PHE:HZ	1:E:159:LEU:HD12	1.83	0.43
1:C:101:ASN:HA	1:C:104:CYS:O	2.18	0.43
1:B:206:LEU:HA	1:B:207:PRO:C	2.38	0.43
1:C:82:GLY:HA2	1:C:148:GLY:H	1.84	0.43
1:A:1:GLU:HG3	1:A:236:VAL:CG2	2.48	0.43
1:F:70:ASP:OD2	1:F:73:ASN:ND2	2.36	0.43
1:G:33:ASN:ND2	1:G:33:ASN:H	2.17	0.43
1:H:166:ILE:O	1:H:191:GLY:HA3	2.19	0.43
1:H:78:LEU:HB3	1:H:142:PHE:CD1	2.54	0.43
1:C:73:ASN:O	1:C:74:LYS:HB2	2.19	0.43
1:D:252:ILE:HA	1:D:253:PRO:HD3	1.97	0.42
1:G:28:ALA:HA	1:G:29:PRO:HD3	1.87	0.42
1:D:264:LEU:HA	1:D:264:LEU:HD13	1.90	0.42
1:G:227:LEU:HD23	1:G:260:TRP:CZ3	2.53	0.42
1:C:260:TRP:CE3	1:C:264:LEU:HD13	2.54	0.42
1:G:240:GLY:O	1:G:243:ALA:HB2	2.18	0.42
1:F:224:SER:CB	2:F:274:HOH:O	2.67	0.42
1:G:221:TRP:CZ3	1:G:223:LYS:HG2	2.54	0.42
1:A:70:ASP:HB3	1:A:75:LEU:HB2	2.00	0.42
1:A:133:ARG:NH1	1:A:133:ARG:HG3	2.31	0.42
1:A:1:GLU:OE2	1:A:233:ASN:O	2.36	0.42
1:H:226:THR:O	1:H:227:LEU:HB2	2.19	0.42
1:C:98:LYS:HD3	1:C:111:ASP:HA	2.00	0.42
1:E:81:ARG:CD	1:E:82:GLY:O	2.67	0.42
1:G:33:ASN:HD22	1:G:33:ASN:H	1.66	0.42
1:F:73:ASN:O	1:F:74:LYS:HB2	2.19	0.42
1:H:116:SER:O	1:H:119:SER:HB2	2.19	0.42
1:A:254:ASP:CG	1:A:256:PRO:HD2	2.40	0.42
1:B:133:ARG:HH11	1:B:133:ARG:HG3	1.85	0.42
1:E:1:GLU:H1	1:E:233:ASN:HA	1.84	0.42
1:D:1:GLU:HG3	1:D:236:VAL:CG2	2.49	0.42
1:H:264:LEU:HD13	1:H:264:LEU:HA	1.82	0.42
1:G:94:ASN:HD21	1:G:96:ASP:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:ASN:HB3	1:F:56:GLU:HB2	2.02	0.42
1:G:254:ASP:OD1	1:G:256:PRO:HD2	2.20	0.42
1:G:25:ASN:HA	1:G:51:PHE:CZ	2.54	0.42
1:B:202:ILE:O	1:B:205:ARG:HB2	2.19	0.42
1:H:223:LYS:HE2	1:H:236:VAL:HG23	2.01	0.42
1:H:206:LEU:HA	1:H:207:PRO:C	2.40	0.42
1:C:33:ASN:HD22	1:C:33:ASN:H	1.68	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:N	2.17	0.42
1:E:133:ARG:HG3	1:E:133:ARG:HH11	1.84	0.42
1:G:164:TYR:HE1	2:G:292:HOH:O	2.03	0.41
1:F:179:ARG:NH1	1:F:179:ARG:HG2	2.35	0.41
1:D:81:ARG:CD	1:D:82:GLY:O	2.68	0.41
1:A:261:TYR:O	1:A:262:PHE:HB2	2.21	0.41
1:F:241:ILE:O	2:F:285:HOH:O	2.22	0.41
1:G:223:LYS:HB2	1:G:223:LYS:HE3	1.77	0.41
1:D:103:ILE:HG13	1:D:103:ILE:H	1.56	0.41
1:E:214:SER:OG	1:E:242:ASP:OD2	2.32	0.41
1:A:223:LYS:HB2	1:A:223:LYS:HE3	1.91	0.41
1:D:179:ARG:HD2	1:D:214:SER:HG	1.82	0.41
1:G:73:ASN:O	1:G:74:LYS:HB2	2.20	0.41
1:F:207:PRO:HG2	1:F:213:TYR:CZ	2.56	0.41
1:G:58:SER:HB2	1:G:63:VAL:O	2.20	0.41
1:B:94:ASN:ND2	1:B:96:ASP:OD2	2.54	0.41
1:E:199:THR:OG1	1:E:200:ASN:N	2.48	0.41
1:D:125:ARG:NE	2:D:319:HOH:O	2.53	0.41
1:H:33:ASN:ND2	1:H:33:ASN:H	2.18	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:D:142:PHE:HZ	1:D:159:LEU:HD12	1.86	0.41
1:F:261:TYR:O	1:F:262:PHE:HB2	2.21	0.41
1:E:208:PRO:HG2	1:E:211:PHE:CD1	2.54	0.41
1:H:1:GLU:HB2	1:H:235:ILE:O	2.21	0.41
1:A:86:ILE:HG21	1:A:258:HIS:CD2	2.56	0.41
1:F:53:TYR:CE1	1:F:127:LYS:HE3	2.57	0.40
1:E:89:TRP:CZ2	1:E:147:LEU:HB2	2.56	0.40
1:D:52:LEU:HD13	1:D:131:ALA:HB2	2.03	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	267/269 (99%)	256 (96%)	10 (4%)	1 (0%)	39	56
1	B	267/269 (99%)	257 (96%)	9 (3%)	1 (0%)	39	56
1	C	267/269 (99%)	255 (96%)	11 (4%)	1 (0%)	39	56
1	D	267/269 (99%)	256 (96%)	8 (3%)	3 (1%)	17	25
1	E	267/269 (99%)	254 (95%)	12 (4%)	1 (0%)	39	56
1	F	267/269 (99%)	256 (96%)	10 (4%)	1 (0%)	39	56
1	G	267/269 (99%)	256 (96%)	10 (4%)	1 (0%)	39	56
1	H	267/269 (99%)	257 (96%)	9 (3%)	1 (0%)	39	56
All	All	2136/2152 (99%)	2047 (96%)	79 (4%)	10 (0%)	34	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	102	ASP
1	A	199	THR

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Mol	Chain	Res	Type
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 (i)

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%)	202 (92%)	18 (8%)	14	21
1	B	220/220 (100%)	199 (90%)	21 (10%)	11	15
1	C	220/220 (100%)	202 (92%)	18 (8%)	14	21
1	D	220/220 (100%)	199 (90%)	21 (10%)	11	15
1	E	220/220 (100%)	201 (91%)	19 (9%)	13	19
1	F	220/220 (100%)	201 (91%)	19 (9%)	13	19
1	G	220/220 (100%)	203 (92%)	17 (8%)	16	24
1	H	220/220 (100%)	200 (91%)	20 (9%)	12	17
All	All	1760/1760 (100%)	1607 (91%)	153 (9%)	13	19

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	33	ASN
1	A	54	SER
1	A	58	SER
1	A	94	ASN
1	A	102	ASP
1	A	118	ARG

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Mol	Chain	Res	Type
1	A	119	SER
1	A	127	LYS
1	A	133	ARG
1	A	146	SER
1	A	162	ASN
1	A	179	ARG
1	A	214	SER
1	A	232	ARG
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	84	ARG
1	B	94	ASN
1	B	98	LYS
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	214	SER
1	B	232	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	84	ARG
1	C	94	ASN
1	C	102	ASP
1	C	118	ARG
1	C	119	SER

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Mol	Chain	Res	Type
1	C	133	ARG
1	C	146	SER
1	C	162	ASN
1	C	179	ARG
1	C	214	SER
1	C	232	ARG
1	C	252	ILE
1	C	264	LEU
1	D	1	GLU
1	D	24	LYS
1	D	33	ASN
1	D	54	SER
1	D	58	SER
1	D	94	ASN
1	D	98	LYS
1	D	102	ASP
1	D	118	ARG
1	D	119	SER
1	D	133	ARG
1	D	146	SER
1	D	162	ASN
1	D	176	VAL
1	D	179	ARG
1	D	214	SER
1	D	232	ARG
1	D	250	PRO
1	D	252	ILE
1	D	264	LEU
1	D	269	LEU
1	E	24	LYS
1	E	33	ASN
1	E	54	SER
1	E	58	SER
1	E	84	ARG
1	E	94	ASN
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

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Mol	Chain	Res	Type
1	E	179	ARG
1	E	214	SER
1	E	232	ARG
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	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	214	SER
1	F	232	ARG
1	F	252	ILE
1	F	264	LEU
1	F	269	LEU
1	G	1	GLU
1	G	33	ASN
1	G	54	SER
1	G	58	SER
1	G	94	ASN
1	G	102	ASP
1	G	118	ARG
1	G	119	SER
1	G	133	ARG
1	G	146	SER
1	G	162	ASN
1	G	179	ARG
1	G	214	SER
1	G	232	ARG
1	G	252	ILE
1	G	264	LEU
1	G	269	LEU

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Mol	Chain	Res	Type
1	H	1	GLU
1	H	33	ASN
1	H	58	SER
1	H	83	SER
1	H	84	ARG
1	H	94	ASN
1	H	102	ASP
1	H	118	ARG
1	H	119	SER
1	H	127	LYS
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	232	ARG
1	H	252	ILE
1	H	264	LEU
1	H	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	247	ASN
1	B	33	ASN
1	C	33	ASN
1	D	33	ASN
1	E	26	ASN
1	E	33	ASN
1	F	33	ASN
1	G	33	ASN
1	H	33	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 carbohydrates 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.