



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 12:35 AM EDT

PDB ID : 4WL2 / pdb_00004wl2
Title : Structure of penicillin V acylase from *Pectobacterium atrosepticum*
Authors : Ramasamy, S.; Avinash, V.S.; Pundle, A.V.; Suresh, C.G.
Deposited on : 2014-10-06
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

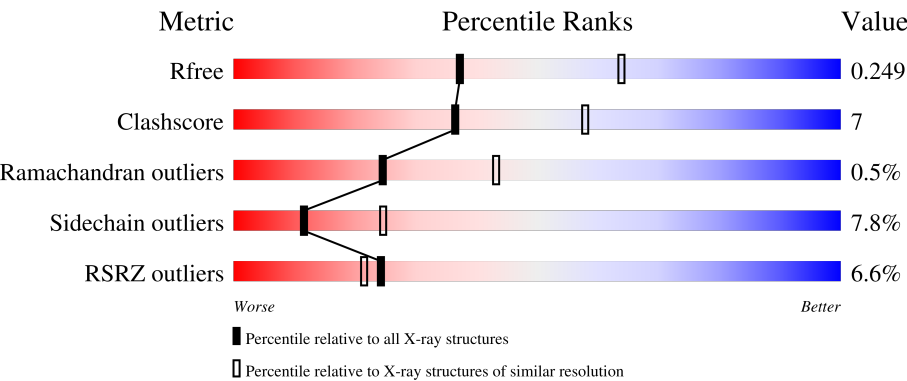
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	355	5% 81%12%...
1	B	355	5% 83%10%...
1	C	355	5% 81%14%..
1	D	355	4% 83%12%...
1	E	355	7% 82%12%...

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Mol	Chain	Length	Quality of chain
1	F	355	8% 85% 10%
1	G	355	5% 83% 11%
1	H	355	12% 81% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21734 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 Putative exported choloylglycine hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	B	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	C	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	D	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	E	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	F	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	G	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	H	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	348	LEU	-	expression tag	UNP Q6D291
A	349	GLU	-	expression tag	UNP Q6D291
A	350	HIS	-	expression tag	UNP Q6D291
A	351	HIS	-	expression tag	UNP Q6D291
A	352	HIS	-	expression tag	UNP Q6D291
A	353	HIS	-	expression tag	UNP Q6D291
A	354	HIS	-	expression tag	UNP Q6D291
A	355	HIS	-	expression tag	UNP Q6D291
B	348	LEU	-	expression tag	UNP Q6D291
B	349	GLU	-	expression tag	UNP Q6D291
B	350	HIS	-	expression tag	UNP Q6D291
B	351	HIS	-	expression tag	UNP Q6D291
B	352	HIS	-	expression tag	UNP Q6D291

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Chain	Residue	Modelled	Actual	Comment	Reference
B	353	HIS	-	expression tag	UNP Q6D291
B	354	HIS	-	expression tag	UNP Q6D291
B	355	HIS	-	expression tag	UNP Q6D291
C	348	LEU	-	expression tag	UNP Q6D291
C	349	GLU	-	expression tag	UNP Q6D291
C	350	HIS	-	expression tag	UNP Q6D291
C	351	HIS	-	expression tag	UNP Q6D291
C	352	HIS	-	expression tag	UNP Q6D291
C	353	HIS	-	expression tag	UNP Q6D291
C	354	HIS	-	expression tag	UNP Q6D291
C	355	HIS	-	expression tag	UNP Q6D291
D	348	LEU	-	expression tag	UNP Q6D291
D	349	GLU	-	expression tag	UNP Q6D291
D	350	HIS	-	expression tag	UNP Q6D291
D	351	HIS	-	expression tag	UNP Q6D291
D	352	HIS	-	expression tag	UNP Q6D291
D	353	HIS	-	expression tag	UNP Q6D291
D	354	HIS	-	expression tag	UNP Q6D291
D	355	HIS	-	expression tag	UNP Q6D291
E	348	LEU	-	expression tag	UNP Q6D291
E	349	GLU	-	expression tag	UNP Q6D291
E	350	HIS	-	expression tag	UNP Q6D291
E	351	HIS	-	expression tag	UNP Q6D291
E	352	HIS	-	expression tag	UNP Q6D291
E	353	HIS	-	expression tag	UNP Q6D291
E	354	HIS	-	expression tag	UNP Q6D291
E	355	HIS	-	expression tag	UNP Q6D291
F	348	LEU	-	expression tag	UNP Q6D291
F	349	GLU	-	expression tag	UNP Q6D291
F	350	HIS	-	expression tag	UNP Q6D291
F	351	HIS	-	expression tag	UNP Q6D291
F	352	HIS	-	expression tag	UNP Q6D291
F	353	HIS	-	expression tag	UNP Q6D291
F	354	HIS	-	expression tag	UNP Q6D291
F	355	HIS	-	expression tag	UNP Q6D291
G	348	LEU	-	expression tag	UNP Q6D291
G	349	GLU	-	expression tag	UNP Q6D291
G	350	HIS	-	expression tag	UNP Q6D291
G	351	HIS	-	expression tag	UNP Q6D291
G	352	HIS	-	expression tag	UNP Q6D291
G	353	HIS	-	expression tag	UNP Q6D291
G	354	HIS	-	expression tag	UNP Q6D291

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Chain	Residue	Modelled	Actual	Comment	Reference
G	355	HIS	-	expression tag	UNP Q6D291
H	348	LEU	-	expression tag	UNP Q6D291
H	349	GLU	-	expression tag	UNP Q6D291
H	350	HIS	-	expression tag	UNP Q6D291
H	351	HIS	-	expression tag	UNP Q6D291
H	352	HIS	-	expression tag	UNP Q6D291
H	353	HIS	-	expression tag	UNP Q6D291
H	354	HIS	-	expression tag	UNP Q6D291
H	355	HIS	-	expression tag	UNP Q6D291

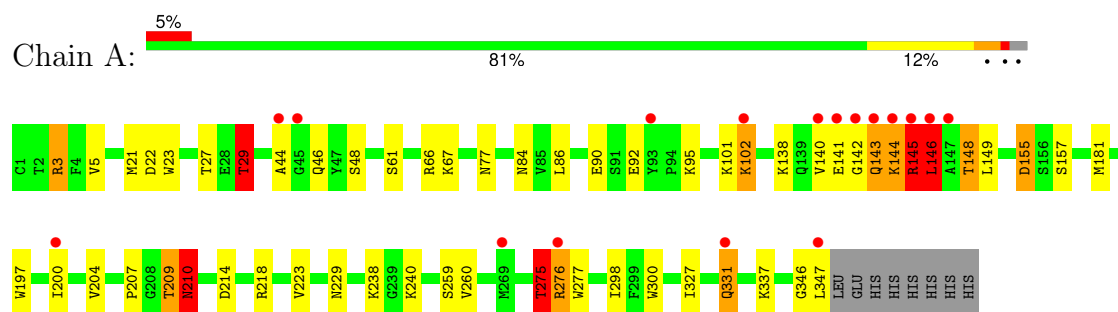
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	3	Total O 3 3	0	0
2	C	5	Total O 5 5	0	0
2	D	7	Total O 7 7	0	0
2	E	5	Total O 5 5	0	0
2	F	2	Total O 2 2	0	0
2	G	9	Total O 9 9	0	0
2	H	4	Total O 4 4	0	0

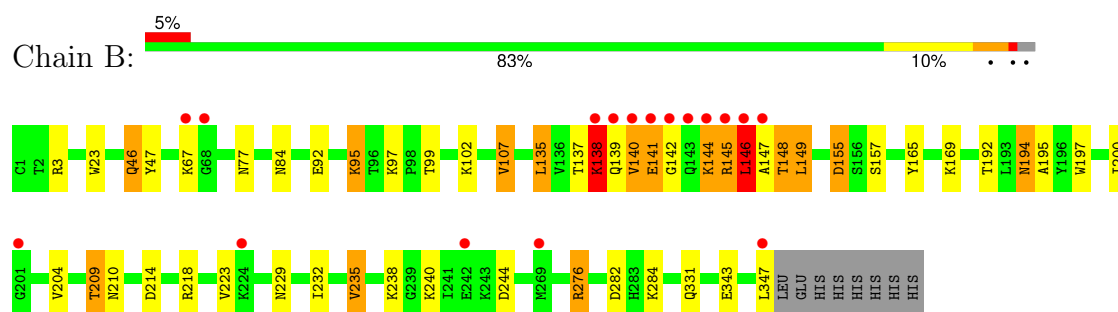
3 Residue-property plots [i](#)

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

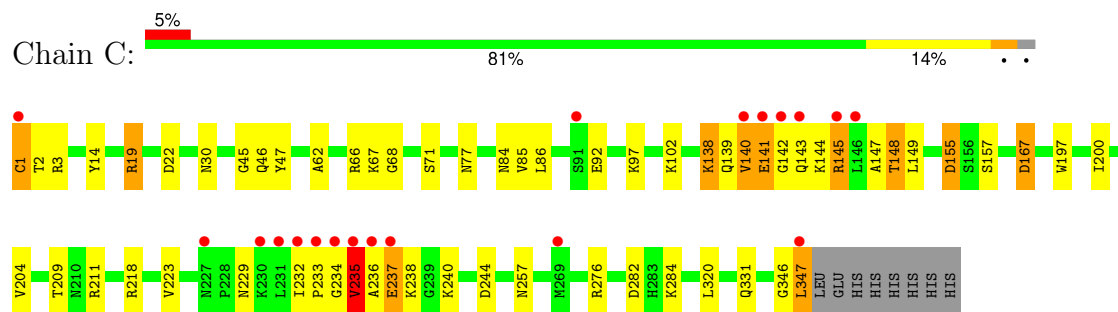
- Molecule 1: Putative exported choloylglycine hydrolase



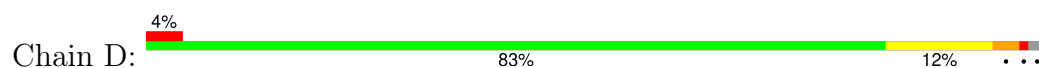
- Molecule 1: Putative exported choloylglycine hydrolase

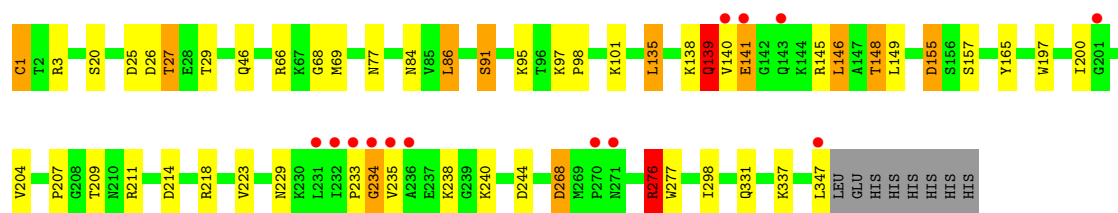


- Molecule 1: Putative exported choloylglycine hydrolase

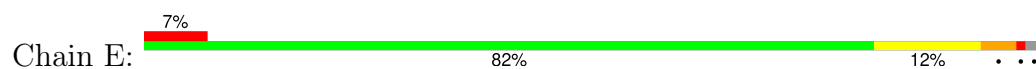


- Molecule 1: Putative exported choloylglycine hydrolase

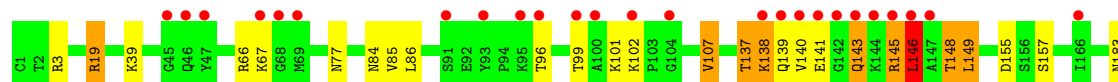
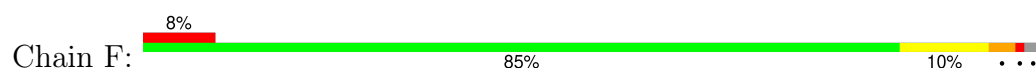




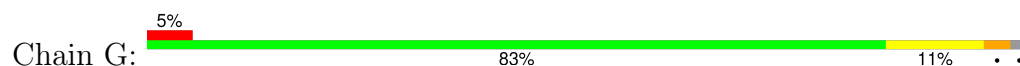
• Molecule 1: Putative exported choloylglycine hydrolase



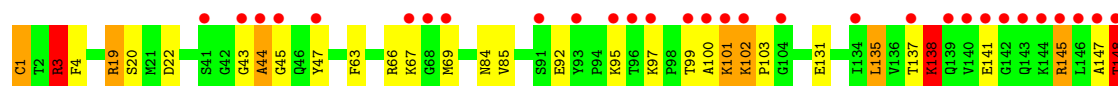
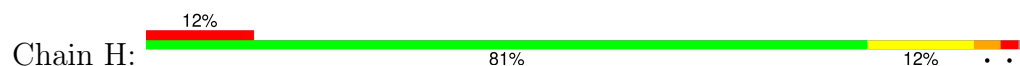
• Molecule 1: Putative exported choloylglycine hydrolase



• Molecule 1: Putative exported choloylglycine hydrolase



• Molecule 1: Putative exported choloylglycine hydrolase



LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.45Å 150.21Å 185.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.43 – 2.50 63.43 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.0 (63.43-2.50) 88.0 (63.43-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.218 , 0.248 0.221 , 0.249	Depositor DCC
R_{free} test set	5077 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21734	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.90	1/2781 (0.0%)	1.05	16/3779 (0.4%)
1	B	0.88	2/2781 (0.1%)	0.97	5/3779 (0.1%)
1	C	1.00	5/2781 (0.2%)	1.01	11/3779 (0.3%)
1	D	0.89	2/2781 (0.1%)	0.98	6/3779 (0.2%)
1	E	0.92	5/2781 (0.2%)	1.15	14/3779 (0.4%)
1	F	0.87	1/2781 (0.0%)	1.13	9/3779 (0.2%)
1	G	0.84	0/2781	0.93	4/3779 (0.1%)
1	H	0.99	5/2781 (0.2%)	1.05	16/3779 (0.4%)
All	All	0.91	21/22248 (0.1%)	1.04	81/30232 (0.3%)

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	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
1	H	0	2
All	All	0	10

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	235	VAL	N-CA	17.11	1.67	1.46
1	H	233	PRO	CA-C	15.69	1.74	1.52
1	H	233	PRO	N-CA	11.59	1.62	1.47
1	E	234	GLY	N-CA	8.05	1.56	1.45
1	H	138	LYS	N-CA	7.05	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	140	VAL	CA-CB	6.63	1.61	1.53
1	E	184	SER	CA-CB	-6.50	1.43	1.53
1	B	138	LYS	N-CA	6.40	1.54	1.46
1	E	233	PRO	CA-C	6.28	1.61	1.52
1	B	140	VAL	N-CA	6.21	1.53	1.46
1	C	235	VAL	CA-CB	6.18	1.62	1.54
1	A	145	ARG	CA-C	6.07	1.55	1.52
1	F	184	SER	CA-CB	-5.53	1.44	1.53
1	E	1	CYS	CA-C	5.45	1.64	1.52
1	C	257	ASN	C-O	-5.29	1.18	1.24
1	H	145	ARG	CA-C	5.24	1.59	1.53
1	C	2	THR	N-CA	5.19	1.52	1.46
1	D	234	GLY	CA-C	5.19	1.59	1.51
1	C	1	CYS	CA-C	5.17	1.63	1.52
1	H	233	PRO	CA-CB	5.09	1.60	1.53
1	D	139	GLN	CA-C	5.07	1.59	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	184	SER	CA-C-N	-25.75	87.65	119.84
1	F	184	SER	C-N-CA	-25.75	87.65	119.84
1	E	184	SER	CA-C-N	-25.00	88.60	119.84
1	E	184	SER	C-N-CA	-25.00	88.60	119.84
1	A	209	THR	N-CA-C	15.81	132.82	113.38
1	B	140	VAL	N-CA-C	14.88	124.52	110.53
1	G	150	HIS	CB-CA-C	-11.05	87.91	111.11
1	C	148	THR	N-CA-C	10.98	126.74	109.07
1	A	3	ARG	NE-CZ-NH2	10.84	128.96	119.20
1	D	148	THR	N-CA-C	9.85	124.93	109.07
1	E	184	SER	N-CA-C	9.62	131.07	109.81
1	F	184	SER	N-CA-C	9.36	130.50	109.81
1	H	233	PRO	N-CA-C	9.36	131.74	112.47
1	B	148	THR	N-CA-C	-9.02	95.98	110.32
1	D	276	ARG	CB-CG-CD	-8.54	91.67	111.30
1	C	235	VAL	N-CA-CB	8.18	124.72	111.23
1	A	209	THR	CB-CA-C	-8.12	95.52	109.65
1	D	276	ARG	CG-CD-NE	8.12	129.85	112.00
1	A	331	GLN	CB-CG-CD	-7.75	99.42	112.60
1	H	145	ARG	N-CA-C	7.75	121.71	109.39
1	H	233	PRO	O-C-N	-7.74	112.19	122.64
1	A	275	THR	N-CA-CB	7.46	120.96	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	233	PRO	CA-C-N	7.27	135.66	121.41
1	H	233	PRO	C-N-CA	7.27	135.66	121.41
1	H	3	ARG	CG-CD-NE	7.27	127.99	112.00
1	C	139	GLN	N-CA-C	-7.19	97.88	109.96
1	C	232	ILE	N-CA-CB	-7.02	101.38	111.21
1	F	284	LYS	CB-CG-CD	6.96	127.32	111.30
1	E	184	SER	C-N-CD	6.72	152.56	125.00
1	A	210	ASN	N-CA-CB	6.72	121.85	110.49
1	A	331	GLN	CB-CA-C	-6.64	100.29	110.26
1	C	237	GLU	N-CA-CB	6.56	120.13	109.69
1	C	232	ILE	CB-CA-C	6.49	123.17	111.36
1	G	150	HIS	CA-CB-CG	6.49	120.28	113.80
1	C	167	ASP	N-CA-CB	-6.37	102.52	112.13
1	E	143	GLN	N-CA-C	6.34	118.74	110.43
1	F	184	SER	C-N-CD	6.34	150.99	125.00
1	E	67	LYS	CA-CB-CG	6.31	126.73	114.10
1	B	146	LEU	N-CA-C	6.14	118.45	108.08
1	A	3	ARG	CB-CG-CD	6.13	125.41	111.30
1	H	337	LYS	CA-CB-CG	6.10	126.31	114.10
1	C	1	CYS	N-CA-C	6.03	127.89	111.00
1	F	184	SER	CB-CA-C	-6.02	98.30	110.17
1	G	148	THR	N-CA-C	-5.97	100.16	109.72
1	A	3	ARG	CG-CD-NE	5.94	125.06	112.00
1	E	1	CYS	N-CA-C	5.90	127.51	111.00
1	E	184	SER	CB-CA-C	-5.89	98.57	110.17
1	H	138	LYS	CB-CG-CD	5.84	124.73	111.30
1	E	140	VAL	N-CA-CB	5.57	117.86	111.39
1	E	232	ILE	N-CA-C	-5.57	102.64	108.15
1	D	155	ASP	CB-CA-C	-5.57	99.28	110.30
1	E	155	ASP	CB-CA-C	-5.57	99.28	110.30
1	H	200	ILE	CA-C-N	-5.56	115.06	120.34
1	H	200	ILE	C-N-CA	-5.56	115.06	120.34
1	H	155	ASP	CB-CA-C	-5.52	99.36	110.30
1	E	47	TYR	N-CA-C	5.52	119.24	111.52
1	H	102	LYS	CB-CG-CD	5.50	123.96	111.30
1	A	46	GLN	N-CA-C	-5.49	106.42	113.23
1	A	276	ARG	CD-NE-CZ	-5.46	116.76	124.40
1	B	155	ASP	CB-CA-C	-5.39	99.64	110.30
1	H	209	THR	N-CA-CB	-5.35	101.90	110.51
1	A	29	THR	N-CA-CB	5.35	118.13	110.06
1	A	155	ASP	CB-CA-C	-5.35	100.19	110.24
1	C	155	ASP	CB-CA-C	-5.35	99.72	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	F	146	LEU	N-CA-C	5.31	116.60	108.42
1	E	199	GLN	CA-CB-CG	5.27	124.64	114.10
1	D	91	SER	CA-CB-OG	-5.26	100.57	111.10
1	H	148	THR	N-CA-CB	-5.23	103.46	111.56
1	E	184	SER	CA-CB-OG	-5.18	100.73	111.10
1	H	1	CYS	N-CA-C	5.16	125.44	111.00
1	C	47	TYR	N-CA-C	5.15	118.73	111.52
1	F	39	LYS	CG-CD-CE	5.14	123.13	111.30
1	C	237	GLU	N-CA-C	-5.11	103.04	110.24
1	B	194	ASN	N-CA-C	5.10	117.74	111.82
1	F	184	SER	CA-CB-OG	-5.05	100.99	111.10
1	G	155	ASP	CB-CA-C	-5.04	100.31	110.30
1	H	331	GLN	CB-CA-C	-5.04	102.03	110.29
1	A	148	THR	N-CA-C	-5.02	102.64	110.42
1	A	327	ILE	N-CA-C	5.01	115.50	108.89
1	D	91	SER	CB-CA-C	-5.01	101.03	109.50

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	346	GLY	Peptide
1	B	137	THR	Peptide
1	C	346	GLY	Peptide
1	D	1	CYS	Peptide
1	D	139	GLN	Peptide
1	E	183	ASN	Peptide
1	F	137	THR	Peptide
1	F	183	ASN	Peptide
1	H	101	LYS	Peptide
1	H	233	PRO	Peptide

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	2711	0	2660	77	0
1	B	2711	0	2660	46	0
1	C	2711	0	2660	34	18
1	D	2711	0	2658	46	18
1	E	2711	0	2660	27	13
1	F	2711	0	2659	22	0
1	G	2711	0	2660	29	0
1	H	2711	0	2660	41	13
2	A	11	0	0	2	0
2	B	3	0	0	0	0
2	C	5	0	0	2	0
2	D	7	0	0	4	0
2	E	5	0	0	0	0
2	F	2	0	0	0	0
2	G	9	0	0	1	0
2	H	4	0	0	0	0
All	All	21734	0	21277	309	31

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 7.

All (309) 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:C:235:VAL:N	1:C:235:VAL:CA	1.67	1.56
1:H:233:PRO:C	1:H:233:PRO:CA	1.74	1.55
1:D:68:GLY:O	1:D:138:LYS:NZ	1.57	1.34
1:D:25:ASP:C	1:D:276:ARG:HH21	1.37	1.31
1:A:3:ARG:NH1	1:A:181:MET:SD	2.03	1.31
1:B:209:THR:HG22	1:B:214:ASP:OD2	1.21	1.28
1:D:26:ASP:N	1:D:276:ARG:HH21	1.36	1.21
1:D:1:CYS:HB3	2:D:406:HOH:O	1.42	1.19
1:A:300:TRP:NE1	1:A:331:GLN:OE1	1.74	1.17
1:B:209:THR:CG2	1:B:214:ASP:OD2	1.94	1.15
1:C:71:SER:O	2:C:404:HOH:O	1.64	1.14
1:A:300:TRP:CD1	1:A:331:GLN:HE22	1.67	1.11
1:A:276:ARG:HG3	1:A:276:ARG:NH1	1.57	1.10
1:A:23:TRP:N	1:A:276:ARG:HH12	1.49	1.10
1:D:25:ASP:C	1:D:276:ARG:NH2	2.11	1.08
1:A:3:ARG:NH1	1:A:181:MET:CE	2.24	1.00
1:D:138:LYS:HE2	1:D:140:VAL:HG11	1.44	0.99
1:A:276:ARG:HG3	1:A:276:ARG:HH11	1.21	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LYS:HD2	2:A:409:HOH:O	1.65	0.97
1:H:302:ASP:HB2	1:H:331:GLN:HE21	1.29	0.96
1:A:23:TRP:N	1:A:276:ARG:NH1	2.16	0.94
1:D:26:ASP:N	1:D:276:ARG:NH2	2.15	0.92
1:A:27:THR:OG1	1:A:29:THR:HG22	1.69	0.91
1:A:300:TRP:CD1	1:A:331:GLN:NE2	2.38	0.91
1:A:260:VAL:H	1:A:275:THR:CG2	1.82	0.91
1:A:276:ARG:HH11	1:A:276:ARG:CG	1.80	0.90
1:A:23:TRP:H	1:A:276:ARG:NH1	1.68	0.89
1:H:233:PRO:C	1:H:233:PRO:HA	1.94	0.88
1:A:29:THR:HB	1:A:61:SER:O	1.74	0.87
1:A:331:GLN:NE2	1:A:331:GLN:HA	1.88	0.87
1:D:1:CYS:CB	2:D:406:HOH:O	2.10	0.86
1:F:204:VAL:HG13	1:G:204:VAL:HG13	1.57	0.86
1:D:140:VAL:O	1:D:140:VAL:HG13	1.76	0.86
1:A:23:TRP:HB3	1:A:276:ARG:CZ	2.04	0.86
1:E:204:VAL:O	1:F:211:ARG:NH2	2.07	0.86
1:A:22:ASP:C	1:A:276:ARG:HH22	1.84	0.86
1:A:23:TRP:H	1:A:276:ARG:HH12	0.86	0.86
1:E:211:ARG:NH2	1:F:204:VAL:O	2.08	0.85
1:D:27:THR:HG23	1:D:29:THR:OG1	1.76	0.85
1:A:3:ARG:HH12	1:A:181:MET:CE	1.86	0.85
1:A:21:MET:HG3	1:A:276:ARG:NH2	1.93	0.83
1:B:204:VAL:O	1:C:211:ARG:NH2	2.11	0.82
1:A:23:TRP:CB	1:A:276:ARG:CZ	2.58	0.81
1:H:220:SER:O	1:H:224:LYS:HD2	1.80	0.80
1:A:23:TRP:HB2	1:A:276:ARG:NH2	1.97	0.79
1:A:29:THR:HG21	1:A:277:TRP:NE1	1.95	0.79
1:H:63:PHE:HB2	1:H:69:MET:O	1.82	0.79
1:B:141:GLU:HB2	1:B:144:LYS:HD3	1.65	0.78
1:D:204:VAL:O	1:G:211:ARG:NH2	2.16	0.78
1:D:1:CYS:CA	2:D:406:HOH:O	2.29	0.78
1:D:139:GLN:HB2	1:D:140:VAL:HA	1.66	0.78
1:B:141:GLU:OE2	1:B:144:LYS:NZ	2.17	0.78
1:D:204:VAL:HG13	1:E:204:VAL:HG13	1.66	0.77
1:H:302:ASP:HB2	1:H:331:GLN:NE2	1.99	0.77
1:C:140:VAL:HG23	1:C:140:VAL:O	1.86	0.76
1:E:184:SER:CB	1:E:212:ALA:CB	2.65	0.75
1:D:1:CYS:N	1:D:86:LEU:HG	2.02	0.74
1:F:184:SER:CB	1:F:212:ALA:CB	2.65	0.74
1:B:141:GLU:CD	1:B:144:LYS:NZ	2.46	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:GLY:O	1:H:44:ALA:HB2	1.88	0.73
1:A:21:MET:HG3	1:A:276:ARG:HH21	1.52	0.72
1:E:138:LYS:HE2	1:E:140:VAL:HG22	1.71	0.72
1:B:139:GLN:HG3	1:B:141:GLU:HB3	1.71	0.71
1:A:300:TRP:NE1	1:A:331:GLN:CD	2.47	0.71
1:B:107:VAL:HG22	1:B:149:LEU:HD11	1.71	0.71
1:D:211:ARG:NH2	1:G:204:VAL:O	2.22	0.71
1:C:204:VAL:HG13	1:H:204:VAL:HG13	1.73	0.71
1:D:69:MET:SD	1:D:141:GLU:HG2	2.32	0.70
1:C:235:VAL:N	1:C:235:VAL:C	2.49	0.70
1:E:107:VAL:HG22	1:E:149:LEU:HD11	1.74	0.70
1:H:102:LYS:CE	1:H:131:GLU:O	2.41	0.69
1:D:138:LYS:HE2	1:D:140:VAL:CG1	2.20	0.69
1:A:21:MET:CG	1:A:276:ARG:HH21	2.04	0.69
1:A:29:THR:HG21	1:A:277:TRP:HE1	1.56	0.69
1:A:22:ASP:OD2	1:A:275:THR:HB	1.92	0.69
1:A:260:VAL:H	1:A:275:THR:HG23	1.56	0.69
1:F:107:VAL:HG22	1:F:149:LEU:HD11	1.74	0.69
1:C:143:GLN:HG3	1:C:145:ARG:H	1.58	0.68
1:C:62:ALA:O	2:C:404:HOH:O	2.11	0.68
1:G:107:VAL:HG22	1:G:149:LEU:HD11	1.74	0.68
1:G:141:GLU:HA	1:G:141:GLU:OE2	1.92	0.67
1:A:23:TRP:CB	1:A:276:ARG:NH2	2.57	0.67
1:A:23:TRP:O	1:A:276:ARG:NH1	2.28	0.67
1:H:102:LYS:HE2	1:H:131:GLU:O	1.94	0.67
1:E:1:CYS:SG	1:E:22:ASP:HB2	2.35	0.67
1:A:140:VAL:HG21	1:A:146:LEU:HD11	1.77	0.66
1:E:138:LYS:CE	1:E:140:VAL:HG22	2.26	0.66
1:E:184:SER:CB	1:E:212:ALA:HB1	2.25	0.66
1:D:25:ASP:CA	1:D:276:ARG:NH2	2.59	0.66
1:B:141:GLU:CD	1:B:144:LYS:HZ2	2.03	0.66
1:B:209:THR:CG2	1:B:214:ASP:CG	2.68	0.66
1:D:1:CYS:H2	1:D:86:LEU:HG	1.58	0.65
1:B:95:LYS:HE3	1:B:95:LYS:HA	1.77	0.65
1:F:184:SER:CB	1:F:212:ALA:HB1	2.27	0.65
1:E:138:LYS:HE2	1:E:140:VAL:CG2	2.27	0.64
1:D:141:GLU:OE1	1:D:141:GLU:HA	1.98	0.64
1:A:27:THR:OG1	1:A:29:THR:CG2	2.44	0.64
1:C:140:VAL:O	1:C:140:VAL:CG2	2.46	0.63
1:F:137:THR:O	1:F:138:LYS:HB2	1.98	0.63
1:D:27:THR:CG2	1:D:29:THR:OG1	2.44	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:CYS:SG	1:H:22:ASP:HB2	2.38	0.63
1:A:204:VAL:HG13	1:B:204:VAL:HG13	1.80	0.63
1:D:140:VAL:O	1:D:140:VAL:CG1	2.45	0.63
1:G:142:GLY:HA3	1:G:143:GLN:HG3	1.81	0.62
1:H:47:TYR:CD2	1:H:99:THR:HA	2.34	0.62
1:D:138:LYS:NZ	1:D:140:VAL:HG12	2.14	0.62
1:E:184:SER:HB2	1:E:212:ALA:CB	2.30	0.62
1:E:184:SER:HB2	1:E:212:ALA:HB1	1.80	0.62
1:F:143:GLN:HG3	1:F:143:GLN:O	2.00	0.62
1:F:184:SER:HB2	1:F:212:ALA:HB1	1.82	0.61
1:A:260:VAL:H	1:A:275:THR:HG22	1.64	0.60
1:F:184:SER:HB2	1:F:212:ALA:CB	2.31	0.60
1:A:145:ARG:C	1:A:146:LEU:HD22	2.26	0.60
1:H:47:TYR:CD2	1:H:100:ALA:N	2.69	0.60
1:A:240:LYS:CD	2:A:409:HOH:O	2.37	0.59
1:D:97:LYS:HG3	1:D:98:PRO:HD2	1.82	0.59
1:H:101:LYS:HA	1:H:103:PRO:HD3	1.83	0.59
1:A:23:TRP:CA	1:A:276:ARG:NH1	2.65	0.59
1:C:45:GLY:N	1:C:347:LEU:C	2.61	0.59
1:C:1:CYS:SG	1:C:22:ASP:HB2	2.42	0.58
1:G:138:LYS:HG3	1:G:347:LEU:HD23	1.84	0.58
1:G:92:GLU:OE1	1:G:167:ASP:N	2.22	0.58
1:H:209:THR:HG22	1:H:211:ARG:H	1.69	0.58
1:C:140:VAL:HG12	1:C:147:ALA:HB2	1.84	0.58
1:D:27:THR:HG21	1:D:277:TRP:HE1	1.69	0.58
1:A:3:ARG:HH12	1:A:181:MET:HE1	1.64	0.57
1:B:139:GLN:HG3	1:B:141:GLU:CB	2.35	0.57
1:D:68:GLY:C	1:D:138:LYS:HZ3	2.00	0.57
1:D:1:CYS:C	2:D:406:HOH:O	2.45	0.56
1:A:3:ARG:CZ	1:A:181:MET:SD	2.90	0.56
1:H:155:ASP:HB3	1:H:157:SER:H	1.70	0.56
1:B:47:TYR:CD2	1:B:99:THR:HA	2.41	0.56
1:F:137:THR:O	1:F:138:LYS:CB	2.52	0.56
1:G:139:GLN:O	1:G:145:ARG:CZ	2.54	0.56
1:F:155:ASP:HB3	1:F:157:SER:H	1.70	0.56
1:A:23:TRP:N	1:A:276:ARG:CZ	2.69	0.55
1:B:145:ARG:O	1:B:146:LEU:HD12	2.07	0.55
1:D:135:LEU:HD12	1:D:165:TYR:CE1	2.42	0.55
1:G:155:ASP:HB3	1:G:157:SER:H	1.70	0.55
1:A:3:ARG:HH21	1:A:5:VAL:HG23	1.72	0.55
1:G:138:LYS:HG3	1:G:347:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ASP:HB3	1:C:157:SER:H	1.72	0.54
1:C:209:THR:O	1:C:218:ARG:NH2	2.40	0.54
1:D:139:GLN:HB2	1:D:140:VAL:CA	2.38	0.54
1:B:209:THR:OG1	1:B:210:ASN:N	2.41	0.54
1:D:139:GLN:CB	1:D:140:VAL:HA	2.36	0.54
1:D:209:THR:O	1:D:218:ARG:NH2	2.41	0.54
1:A:23:TRP:N	1:A:276:ARG:HH22	2.06	0.54
1:A:21:MET:SD	1:A:276:ARG:NH2	2.80	0.54
1:B:141:GLU:OE1	1:B:142:GLY:N	2.40	0.54
1:H:137:THR:HG23	1:H:138:LYS:CG	2.37	0.54
1:F:209:THR:O	1:F:218:ARG:NH2	2.41	0.54
1:A:300:TRP:CE2	1:A:331:GLN:OE1	2.57	0.54
1:G:102:LYS:HD2	1:G:134:ILE:HG12	1.90	0.53
1:E:135:LEU:HD12	1:E:165:TYR:CE1	2.43	0.53
1:E:209:THR:O	1:E:218:ARG:NH2	2.42	0.53
1:A:229:ASN:OD1	1:A:238:LYS:HE3	2.09	0.53
1:C:229:ASN:OD1	1:C:238:LYS:HE3	2.09	0.53
1:B:144:LYS:HB2	1:B:145:ARG:HA	1.90	0.53
1:G:209:THR:O	1:G:218:ARG:NH2	2.41	0.53
1:F:229:ASN:OD1	1:F:238:LYS:HE3	2.09	0.52
1:A:140:VAL:CG2	1:A:146:LEU:HD11	2.39	0.52
1:B:229:ASN:OD1	1:B:238:LYS:HE3	2.09	0.52
1:G:229:ASN:OD1	1:G:238:LYS:HE3	2.09	0.52
1:B:47:TYR:HD2	1:B:99:THR:HA	1.73	0.52
1:B:197:TRP:O	1:B:200:ILE:O	2.28	0.52
1:H:209:THR:HB	1:H:214:ASP:OD2	2.10	0.52
1:A:155:ASP:HB3	1:A:157:SER:H	1.74	0.52
1:A:259:SER:HB3	1:A:275:THR:CG2	2.40	0.52
1:B:135:LEU:HD12	1:B:165:TYR:CE1	2.44	0.52
1:B:155:ASP:HB3	1:B:157:SER:H	1.74	0.51
1:B:209:THR:O	1:B:218:ARG:NH2	2.43	0.51
1:E:229:ASN:OD1	1:E:238:LYS:HE3	2.10	0.51
1:G:197:TRP:O	1:G:200:ILE:O	2.28	0.51
1:H:197:TRP:O	1:H:200:ILE:O	2.29	0.51
1:H:209:THR:O	1:H:218:ARG:NH2	2.44	0.51
1:A:197:TRP:O	1:A:200:ILE:O	2.28	0.51
1:B:145:ARG:O	1:B:145:ARG:HG2	2.09	0.51
1:D:197:TRP:O	1:D:200:ILE:O	2.28	0.51
1:D:229:ASN:OD1	1:D:238:LYS:HE3	2.09	0.51
1:C:197:TRP:O	1:C:200:ILE:O	2.29	0.51
1:A:23:TRP:N	1:A:276:ARG:NH2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:LEU:HD12	1:H:165:TYR:CE1	2.45	0.51
1:F:197:TRP:O	1:F:200:ILE:O	2.28	0.51
1:B:138:LYS:HG3	1:B:139:GLN:N	2.26	0.51
1:E:1:CYS:HB2	1:E:22:ASP:CG	2.36	0.51
1:E:197:TRP:O	1:E:200:ILE:O	2.28	0.51
1:D:155:ASP:HB3	1:D:157:SER:H	1.76	0.51
1:H:233:PRO:C	1:H:233:PRO:CB	2.78	0.51
1:D:1:CYS:H1	1:D:86:LEU:HG	1.76	0.50
1:F:138:LYS:HG3	1:F:139:GLN:N	2.26	0.50
1:C:240:LYS:NZ	1:C:244:ASP:OD1	2.43	0.50
1:C:45:GLY:H	1:C:347:LEU:C	2.19	0.50
1:D:138:LYS:CE	1:D:140:VAL:CG1	2.87	0.50
1:H:240:LYS:NZ	1:H:244:ASP:OD1	2.42	0.50
1:E:9:PRO:HD2	1:E:227:ASN:ND2	2.27	0.50
1:A:298:ILE:HG22	1:H:298:ILE:HG22	1.94	0.49
1:G:140:VAL:O	1:G:141:GLU:HG2	2.12	0.49
1:B:209:THR:HG23	1:B:214:ASP:CG	2.38	0.49
1:C:141:GLU:HA	1:C:142:GLY:C	2.38	0.49
1:D:1:CYS:HB2	1:D:20:SER:O	2.13	0.49
1:F:146:LEU:HD23	1:F:148:THR:OG1	2.11	0.49
1:G:240:LYS:NZ	1:G:244:ASP:OD1	2.44	0.49
1:E:102:LYS:HD2	1:E:134:ILE:HG12	1.95	0.49
1:A:3:ARG:NH1	1:A:181:MET:HE3	2.24	0.48
1:A:300:TRP:NE1	1:A:331:GLN:NE2	2.60	0.48
1:D:268:ASP:OD1	1:D:268:ASP:N	2.46	0.48
1:A:3:ARG:NH1	1:A:181:MET:HE1	2.20	0.48
1:A:140:VAL:CB	1:A:146:LEU:HD11	2.44	0.48
1:H:1:CYS:HB2	1:H:22:ASP:CG	2.39	0.48
1:B:232:ILE:HB	1:B:235:VAL:HG13	1.96	0.47
1:E:240:LYS:NZ	1:E:244:ASP:OD1	2.43	0.47
1:B:144:LYS:CB	1:B:145:ARG:HA	2.43	0.47
1:D:298:ILE:HG22	1:G:298:ILE:HG22	1.96	0.47
1:E:155:ASP:HB3	1:E:157:SER:H	1.80	0.47
1:H:137:THR:HG23	1:H:138:LYS:HG3	1.96	0.47
1:H:63:PHE:CB	1:H:69:MET:O	2.56	0.47
1:H:147:ALA:C	1:H:148:THR:OG1	2.56	0.47
1:B:95:LYS:HA	1:B:95:LYS:CE	2.39	0.47
1:F:19:ARG:NH2	1:F:85:VAL:O	2.47	0.47
1:A:260:VAL:N	1:A:275:THR:HG23	2.28	0.47
1:A:209:THR:O	1:A:210:ASN:CB	2.63	0.47
1:A:259:SER:HB3	1:A:275:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:O	1:A:146:LEU:HD22	2.15	0.47
1:G:138:LYS:HE3	1:G:347:LEU:HA	1.97	0.47
1:B:46:GLN:OE1	1:B:47:TYR:CE1	2.69	0.46
1:B:169:LYS:HD2	1:B:169:LYS:N	2.31	0.46
1:C:140:VAL:CG2	1:C:145:ARG:HE	2.29	0.46
1:C:234:GLY:C	1:C:235:VAL:CA	2.75	0.46
1:B:232:ILE:O	1:B:235:VAL:HG13	2.16	0.46
1:C:237:GLU:HG3	1:C:238:LYS:O	2.15	0.46
1:H:69:MET:O	1:H:69:MET:HG3	2.16	0.46
1:A:259:SER:CB	1:A:275:THR:HG21	2.46	0.46
1:A:300:TRP:CD1	1:A:331:GLN:CD	2.88	0.46
1:D:138:LYS:NZ	1:D:140:VAL:CG1	2.78	0.46
1:B:145:ARG:O	1:B:145:ARG:CG	2.63	0.46
1:E:282:ASP:OD1	1:E:282:ASP:C	2.58	0.46
1:A:102:LYS:HA	1:A:102:LYS:HD3	1.60	0.45
1:D:240:LYS:NZ	1:D:244:ASP:OD1	2.42	0.45
1:H:19:ARG:NH2	1:H:85:VAL:O	2.48	0.45
1:A:143:GLN:HA	1:A:144:LYS:HA	1.81	0.45
1:G:19:ARG:NH2	1:G:85:VAL:O	2.49	0.45
1:H:47:TYR:CD2	1:H:99:THR:CA	3.00	0.45
1:A:300:TRP:CG	1:A:331:GLN:HE22	2.24	0.45
1:C:282:ASP:OD1	1:C:282:ASP:C	2.60	0.45
1:E:1:CYS:HB2	1:E:22:ASP:OD1	2.17	0.45
1:H:47:TYR:HD2	1:H:99:THR:HA	1.78	0.45
1:F:240:LYS:NZ	1:F:244:ASP:OD1	2.44	0.45
1:A:29:THR:CG2	1:A:277:TRP:HE1	2.27	0.44
1:G:140:VAL:O	1:G:141:GLU:CB	2.65	0.44
1:A:260:VAL:N	1:A:275:THR:CG2	2.66	0.44
1:B:284:LYS:HA	1:B:284:LYS:HD3	1.83	0.44
1:E:231:LEU:O	1:E:232:ILE:HD13	2.17	0.44
1:D:146:LEU:HD12	1:D:146:LEU:HA	1.75	0.44
1:C:19:ARG:NH2	1:C:85:VAL:O	2.50	0.44
1:H:282:ASP:C	1:H:282:ASP:OD1	2.61	0.44
1:C:1:CYS:HB2	1:C:22:ASP:CG	2.43	0.44
1:C:77:ASN:OD1	1:C:77:ASN:C	2.60	0.44
1:D:77:ASN:OD1	1:D:77:ASN:C	2.61	0.44
1:G:142:GLY:HA2	1:G:145:ARG:HH21	1.83	0.43
1:G:225:ASN:HB3	2:G:408:HOH:O	2.17	0.43
1:C:140:VAL:HG21	1:C:145:ARG:HE	1.83	0.43
1:B:144:LYS:HZ3	1:B:146:LEU:N	2.17	0.43
1:B:240:LYS:NZ	1:B:244:ASP:OD1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ASP:OD1	1:B:282:ASP:C	2.61	0.43
1:A:240:LYS:HB2	1:A:240:LYS:HE3	1.78	0.43
1:B:192:THR:OG1	1:H:195:ALA:HB1	2.18	0.43
1:C:3:ARG:HD3	1:C:3:ARG:C	2.44	0.43
1:H:1:CYS:HB2	1:H:22:ASP:OD1	2.18	0.43
1:C:233:PRO:HA	1:C:234:GLY:HA2	1.67	0.42
1:F:145:ARG:HB2	1:F:146:LEU:HD13	2.01	0.42
1:A:21:MET:CG	1:A:276:ARG:NH2	2.66	0.42
1:C:14:TYR:OH	1:C:282:ASP:OD2	2.29	0.42
1:G:23:TRP:O	1:G:276:ARG:HD2	2.20	0.42
1:C:68:GLY:O	1:C:138:LYS:HE2	2.20	0.42
1:H:3:ARG:HG2	1:H:4:PHE:N	2.35	0.42
1:C:138:LYS:HB3	1:C:138:LYS:HE3	1.79	0.42
1:E:23:TRP:O	1:E:276:ARG:HD2	2.18	0.42
1:G:143:GLN:HA	1:G:144:LYS:HA	1.85	0.42
1:A:142:GLY:O	1:A:143:GLN:HB2	2.19	0.42
1:A:207:PRO:HB2	1:A:214:ASP:CG	2.45	0.42
1:B:194:ASN:O	1:B:195:ALA:C	2.61	0.42
1:H:302:ASP:CB	1:H:331:GLN:NE2	2.78	0.42
1:B:47:TYR:HD2	1:B:99:THR:CA	2.32	0.41
1:B:139:GLN:CG	1:B:144:LYS:HE3	2.50	0.41
1:A:77:ASN:OD1	1:A:77:ASN:C	2.63	0.41
1:A:259:SER:HA	1:A:275:THR:HG21	2.01	0.41
1:G:138:LYS:CG	1:G:139:GLN:H	2.33	0.41
1:H:300:TRP:HE1	1:H:331:GLN:NE2	2.18	0.41
1:B:232:ILE:HB	1:B:235:VAL:CG1	2.50	0.41
1:F:302:ASP:H	1:F:331:GLN:NE2	2.18	0.41
1:B:192:THR:OG1	1:H:195:ALA:CB	2.69	0.41
1:D:25:ASP:HA	1:D:276:ARG:NH2	2.31	0.41
1:E:1:CYS:HB2	1:E:22:ASP:HB2	2.03	0.41
1:H:44:ALA:HA	1:H:45:GLY:HA2	1.77	0.41
1:E:31:LEU:HB2	1:E:318:LEU:HB3	2.02	0.41
1:F:77:ASN:OD1	1:F:77:ASN:C	2.64	0.41
1:G:207:PRO:HB2	1:G:214:ASP:CG	2.46	0.41
1:G:284:LYS:HA	1:G:284:LYS:HD3	1.87	0.41
1:B:77:ASN:OD1	1:B:77:ASN:C	2.64	0.41
1:A:29:THR:CG2	1:A:277:TRP:NE1	2.76	0.40
1:A:44:ALA:O	1:A:48:SER:HB3	2.21	0.40
1:C:30:ASN:ND2	1:C:320:LEU:H	2.19	0.40
1:G:77:ASN:OD1	1:G:77:ASN:C	2.64	0.40
1:B:23:TRP:O	1:B:276:ARG:HD2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:ARG:HD2	1:H:20:SER:C	2.46	0.40
1:A:44:ALA:H	1:A:48:SER:HB2	1.87	0.40
1:C:284:LYS:HA	1:C:284:LYS:HD3	1.90	0.40
1:D:207:PRO:HB2	1:D:214:ASP:CG	2.46	0.40

All (31) 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)
1:C:235:VAL:N	1:D:234:GLY:C[4_555]	0.89	1.31
1:C:235:VAL:N	1:D:234:GLY:CA[4_555]	1.01	1.19
1:C:234:GLY:O	1:D:234:GLY:O[4_555]	1.05	1.15
1:E:233:PRO:C	1:H:233:PRO:N[4_455]	1.06	1.14
1:E:233:PRO:O	1:H:233:PRO:N[4_455]	1.13	1.07
1:E:232:ILE:O	1:H:233:PRO:O[4_455]	1.22	0.98
1:C:234:GLY:C	1:D:234:GLY:C[4_555]	1.32	0.88
1:C:234:GLY:N	1:D:233:PRO:O[4_555]	1.54	0.66
1:E:233:PRO:O	1:H:233:PRO:CB[4_455]	1.57	0.63
1:C:235:VAL:N	1:D:235:VAL:N[4_555]	1.60	0.60
1:C:234:GLY:C	1:D:234:GLY:O[4_555]	1.64	0.56
1:E:232:ILE:O	1:H:234:GLY:N[4_455]	1.70	0.50
1:C:233:PRO:O	1:D:233:PRO:O[4_555]	1.71	0.49
1:E:234:GLY:N	1:H:232:ILE:O[4_455]	1.71	0.49
1:E:233:PRO:O	1:H:233:PRO:CG[4_455]	1.73	0.47
1:C:234:GLY:O	1:D:234:GLY:C[4_555]	1.74	0.46
1:C:235:VAL:C	1:D:234:GLY:O[4_555]	1.76	0.44
1:E:234:GLY:N	1:H:233:PRO:N[4_455]	1.80	0.40
1:C:235:VAL:N	1:D:234:GLY:N[4_555]	1.81	0.39
1:C:235:VAL:CA	1:D:234:GLY:CA[4_555]	1.82	0.38
1:E:233:PRO:C	1:H:232:ILE:C[4_455]	1.88	0.32
1:C:234:GLY:C	1:D:234:GLY:CA[4_555]	1.92	0.28
1:E:234:GLY:N	1:H:232:ILE:C[4_455]	1.93	0.27
1:C:235:VAL:CA	1:D:235:VAL:N[4_555]	1.97	0.23
1:C:235:VAL:C	1:D:234:GLY:C[4_555]	1.98	0.22
1:C:235:VAL:N	1:D:234:GLY:O[4_555]	2.03	0.17
1:E:233:PRO:C	1:H:233:PRO:C[4_455]	2.09	0.11
1:C:236:ALA:N	1:D:234:GLY:O[4_555]	2.10	0.10
1:E:234:GLY:CA	1:H:233:PRO:CA[4_455]	2.13	0.07
1:E:232:ILE:C	1:H:233:PRO:O[4_455]	2.16	0.04
1:C:234:GLY:C	1:D:235:VAL:N[4_555]	2.19	0.01

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	345/355 (97%)	334 (97%)	8 (2%)	3 (1%)	14	27
1	B	345/355 (97%)	336 (97%)	7 (2%)	2 (1%)	21	38
1	C	345/355 (97%)	338 (98%)	6 (2%)	1 (0%)	36	55
1	D	345/355 (97%)	338 (98%)	7 (2%)	0	100	100
1	E	345/355 (97%)	337 (98%)	6 (2%)	2 (1%)	21	38
1	F	345/355 (97%)	336 (97%)	7 (2%)	2 (1%)	21	38
1	G	345/355 (97%)	337 (98%)	7 (2%)	1 (0%)	36	55
1	H	345/355 (97%)	332 (96%)	11 (3%)	2 (1%)	21	38
All	All	2760/2840 (97%)	2688 (97%)	59 (2%)	13 (0%)	24	43

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	147	ALA
1	H	138	LYS
1	H	44	ALA
1	A	143	GLN
1	A	210	ASN
1	B	138	LYS
1	C	235	VAL
1	G	141	GLU
1	A	146	LEU
1	E	184	SER
1	F	184	SER
1	F	185	PRO
1	E	185	PRO

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	289/297 (97%)	267 (92%)	22 (8%)	12	26
1	B	289/297 (97%)	264 (91%)	25 (9%)	9	21
1	C	289/297 (97%)	268 (93%)	21 (7%)	13	27
1	D	289/297 (97%)	268 (93%)	21 (7%)	13	27
1	E	289/297 (97%)	264 (91%)	25 (9%)	9	21
1	F	289/297 (97%)	265 (92%)	24 (8%)	10	22
1	G	289/297 (97%)	267 (92%)	22 (8%)	12	26
1	H	289/297 (97%)	268 (93%)	21 (7%)	13	27
All	All	2312/2376 (97%)	2131 (92%)	181 (8%)	11	24

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	66	ARG
1	A	67	LYS
1	A	84	ASN
1	A	86	LEU
1	A	90	GLU
1	A	92	GLU
1	A	95	LYS
1	A	101	LYS
1	A	102	LYS
1	A	138	LYS
1	A	141	GLU
1	A	144	LYS
1	A	145	ARG
1	A	146	LEU
1	A	148	THR
1	A	149	LEU
1	A	218	ARG
1	A	223	VAL

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Mol	Chain	Res	Type
1	A	275	THR
1	A	337	LYS
1	A	347	LEU
1	B	3	ARG
1	B	46	GLN
1	B	67	LYS
1	B	84	ASN
1	B	92	GLU
1	B	95	LYS
1	B	97	LYS
1	B	102	LYS
1	B	107	VAL
1	B	135	LEU
1	B	138	LYS
1	B	140	VAL
1	B	141	GLU
1	B	144	LYS
1	B	145	ARG
1	B	146	LEU
1	B	148	THR
1	B	149	LEU
1	B	209	THR
1	B	223	VAL
1	B	235	VAL
1	B	276	ARG
1	B	331	GLN
1	B	343	GLU
1	B	347	LEU
1	C	19	ARG
1	C	46	GLN
1	C	66	ARG
1	C	67	LYS
1	C	84	ASN
1	C	86	LEU
1	C	92	GLU
1	C	97	LYS
1	C	102	LYS
1	C	138	LYS
1	C	140	VAL
1	C	141	GLU
1	C	144	LYS
1	C	145	ARG

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Mol	Chain	Res	Type
1	C	148	THR
1	C	149	LEU
1	C	167	ASP
1	C	223	VAL
1	C	276	ARG
1	C	331	GLN
1	C	347	LEU
1	D	3	ARG
1	D	27	THR
1	D	46	GLN
1	D	66	ARG
1	D	84	ASN
1	D	86	LEU
1	D	91	SER
1	D	95	LYS
1	D	101	LYS
1	D	135	LEU
1	D	141	GLU
1	D	145	ARG
1	D	146	LEU
1	D	148	THR
1	D	149	LEU
1	D	223	VAL
1	D	268	ASP
1	D	276	ARG
1	D	331	GLN
1	D	337	LYS
1	D	347	LEU
1	E	3	ARG
1	E	31	LEU
1	E	46	GLN
1	E	66	ARG
1	E	84	ASN
1	E	90	GLU
1	E	95	LYS
1	E	102	LYS
1	E	107	VAL
1	E	135	LEU
1	E	139	GLN
1	E	140	VAL
1	E	141	GLU
1	E	143	GLN

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Mol	Chain	Res	Type
1	E	144	LYS
1	E	146	LEU
1	E	148	THR
1	E	149	LEU
1	E	199	GLN
1	E	223	VAL
1	E	268	ASP
1	E	276	ARG
1	E	331	GLN
1	E	337	LYS
1	E	347	LEU
1	F	3	ARG
1	F	19	ARG
1	F	66	ARG
1	F	67	LYS
1	F	84	ASN
1	F	86	LEU
1	F	96	THR
1	F	99	THR
1	F	101	LYS
1	F	102	LYS
1	F	107	VAL
1	F	138	LYS
1	F	140	VAL
1	F	141	GLU
1	F	143	GLN
1	F	145	ARG
1	F	146	LEU
1	F	148	THR
1	F	149	LEU
1	F	223	VAL
1	F	276	ARG
1	F	284	LYS
1	F	331	GLN
1	F	337	LYS
1	G	3	ARG
1	G	19	ARG
1	G	46	GLN
1	G	66	ARG
1	G	67	LYS
1	G	84	ASN
1	G	86	LEU

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Mol	Chain	Res	Type
1	G	92	GLU
1	G	95	LYS
1	G	101	LYS
1	G	102	LYS
1	G	107	VAL
1	G	143	GLN
1	G	144	LYS
1	G	145	ARG
1	G	148	THR
1	G	149	LEU
1	G	223	VAL
1	G	276	ARG
1	G	331	GLN
1	G	337	LYS
1	G	343	GLU
1	H	3	ARG
1	H	19	ARG
1	H	66	ARG
1	H	67	LYS
1	H	84	ASN
1	H	92	GLU
1	H	95	LYS
1	H	97	LYS
1	H	135	LEU
1	H	141	GLU
1	H	145	ARG
1	H	148	THR
1	H	149	LEU
1	H	209	THR
1	H	223	VAL
1	H	224	LYS
1	H	276	ARG
1	H	329	SER
1	H	331	GLN
1	H	337	LYS
1	H	347	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	B	150	HIS

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Mol	Chain	Res	Type
1	B	170	GLN
1	B	331	GLN
1	C	30	ASN
1	C	84	ASN
1	C	139	GLN
1	C	170	GLN
1	C	179	GLN
1	C	331	GLN
1	D	112	GLN
1	D	139	GLN
1	D	170	GLN
1	D	173	HIS
1	D	227	ASN
1	D	331	GLN
1	E	112	GLN
1	E	170	GLN
1	E	210	ASN
1	E	331	GLN
1	F	170	GLN
1	F	225	ASN
1	G	36	GLN
1	G	170	GLN
1	G	331	GLN
1	H	36	GLN
1	H	170	GLN
1	H	179	GLN
1	H	331	GLN
1	H	340	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	347/355 (97%)	0.22	17 (4%)	35	31	19, 34, 75, 172	0
1	B	347/355 (97%)	0.31	17 (4%)	35	31	18, 36, 77, 175	0
1	C	347/355 (97%)	0.18	19 (5%)	30	27	20, 34, 73, 201	0
1	D	347/355 (97%)	0.18	13 (3%)	45	40	18, 33, 69, 128	0
1	E	347/355 (97%)	0.29	26 (7%)	20	18	18, 34, 81, 182	0
1	F	347/355 (97%)	0.50	30 (8%)	16	14	20, 39, 83, 163	0
1	G	347/355 (97%)	0.30	19 (5%)	30	27	21, 39, 75, 199	0
1	H	347/355 (97%)	0.57	41 (11%)	9	7	21, 41, 86, 149	0
All	All	2776/2840 (97%)	0.32	182 (6%)	24	21	18, 36, 80, 201	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	347	LEU	8.6
1	E	347	LEU	8.5
1	A	347	LEU	8.1
1	D	140	VAL	8.0
1	A	147	ALA	7.9
1	B	146	LEU	7.8
1	C	235	VAL	7.7
1	E	140	VAL	7.7
1	C	347	LEU	7.1
1	B	140	VAL	7.0
1	F	347	LEU	6.9
1	F	147	ALA	6.9
1	E	233	PRO	6.7
1	C	232	ILE	6.6
1	G	347	LEU	6.6
1	G	147	ALA	6.5

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Mol	Chain	Res	Type	RSRZ
1	H	140	VAL	6.5
1	H	347	LEU	6.5
1	G	146	LEU	6.4
1	A	146	LEU	6.2
1	B	347	LEU	6.2
1	E	146	LEU	6.2
1	C	233	PRO	6.2
1	H	146	LEU	6.1
1	H	147	ALA	6.1
1	F	140	VAL	5.9
1	C	236	ALA	5.8
1	G	140	VAL	5.6
1	F	146	LEU	5.5
1	H	232	ILE	5.3
1	F	184	SER	5.2
1	E	232	ILE	5.1
1	D	233	PRO	5.1
1	D	232	ILE	5.1
1	A	140	VAL	5.1
1	H	233	PRO	5.0
1	B	147	ALA	4.8
1	E	69	MET	4.7
1	B	145	ARG	4.7
1	G	144	LYS	4.6
1	E	1	CYS	4.6
1	E	147	ALA	4.6
1	D	235	VAL	4.5
1	E	234	GLY	4.5
1	H	234	GLY	4.5
1	E	184	SER	4.4
1	E	142	GLY	4.3
1	C	146	LEU	4.3
1	A	276	ARG	4.3
1	F	142	GLY	4.2
1	E	141	GLU	4.2
1	B	142	GLY	4.2
1	F	144	LYS	4.2
1	F	104	GLY	4.2
1	H	44	ALA	4.2
1	H	144	LYS	4.1
1	E	230	LYS	4.1
1	E	143	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	143	GLN	4.0
1	A	142	GLY	3.9
1	F	143	GLN	3.9
1	C	234	GLY	3.9
1	H	235	VAL	3.9
1	A	331	GLN	3.8
1	C	231	LEU	3.8
1	H	69	MET	3.7
1	B	144	LYS	3.7
1	H	145	ARG	3.6
1	B	139	GLN	3.6
1	A	144	LYS	3.5
1	C	230	LYS	3.5
1	H	201	GLY	3.5
1	G	143	GLN	3.4
1	H	269	MET	3.4
1	C	1	CYS	3.4
1	A	143	GLN	3.4
1	H	101	LYS	3.4
1	D	234	GLY	3.4
1	G	139	GLN	3.4
1	F	99	THR	3.4
1	E	145	ARG	3.3
1	F	141	GLU	3.3
1	H	139	GLN	3.3
1	H	96	THR	3.3
1	H	41	SER	3.2
1	G	145	ARG	3.2
1	F	102	LYS	3.2
1	B	269	MET	3.2
1	H	91	SER	3.1
1	B	141	GLU	3.1
1	D	231	LEU	3.1
1	G	269	MET	3.1
1	C	140	VAL	3.1
1	F	45	GLY	3.1
1	H	142	GLY	3.1
1	G	138	LYS	3.1
1	A	141	GLU	3.1
1	D	141	GLU	3.1
1	B	67	LYS	3.0
1	A	44	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	47	TYR	3.0
1	G	141	GLU	3.0
1	C	145	ARG	2.9
1	B	201	GLY	2.9
1	G	142	GLY	2.9
1	F	96	THR	2.9
1	B	138	LYS	2.9
1	H	143	GLN	2.9
1	A	45	GLY	2.9
1	A	145	ARG	2.8
1	C	141	GLU	2.8
1	F	166	ILE	2.8
1	H	137	THR	2.8
1	E	236	ALA	2.8
1	G	150	HIS	2.7
1	H	68	GLY	2.7
1	E	235	VAL	2.7
1	E	144	LYS	2.7
1	F	69	MET	2.7
1	F	95	LYS	2.6
1	F	145	ARG	2.6
1	F	201	GLY	2.6
1	D	236	ALA	2.6
1	E	346	GLY	2.5
1	H	231	LEU	2.5
1	G	337	LYS	2.5
1	E	269	MET	2.5
1	D	270	PRO	2.5
1	H	102	LYS	2.5
1	D	271	ASN	2.5
1	B	68	GLY	2.5
1	A	102	LYS	2.4
1	H	331	GLN	2.4
1	F	68	GLY	2.4
1	D	143	GLN	2.4
1	C	91	SER	2.4
1	F	138	LYS	2.4
1	H	104	GLY	2.4
1	F	100	ALA	2.4
1	F	91	SER	2.3
1	G	91	SER	2.3
1	H	93	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	338	PRO	2.3
1	F	139	GLN	2.3
1	H	134	ILE	2.3
1	F	67	LYS	2.3
1	D	201	GLY	2.3
1	G	67	LYS	2.3
1	E	91	SER	2.2
1	H	97	LYS	2.2
1	C	237	GLU	2.2
1	H	141	GLU	2.2
1	C	227	ASN	2.2
1	E	93	TYR	2.2
1	A	269	MET	2.2
1	A	93	TYR	2.2
1	H	67	LYS	2.2
1	H	95	LYS	2.2
1	C	143	GLN	2.2
1	E	47	TYR	2.2
1	G	230	LYS	2.2
1	E	231	LEU	2.1
1	G	101	LYS	2.1
1	H	43	GLY	2.1
1	H	99	THR	2.1
1	F	93	TYR	2.1
1	H	47	TYR	2.1
1	B	224	LYS	2.1
1	F	269	MET	2.1
1	C	142	GLY	2.1
1	F	266	LEU	2.1
1	E	268	ASP	2.1
1	H	100	ALA	2.1
1	H	45	GLY	2.1
1	B	242	GLU	2.1
1	F	46	GLN	2.0
1	E	227	ASN	2.0
1	A	200	ILE	2.0
1	G	137	THR	2.0
1	H	148	THR	2.0
1	C	269	MET	2.0
1	H	155	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.