



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 10:44 AM UTC

PDB ID : 1DZB / pdb_00001dzb
Title : Crystal structure of phage library-derived single-chain Fv fragment 1F9 in complex with turkey egg-white lysozyme
Authors : Ay, J.; Keitel, T.; Kuettner, G.; Wessner, H.; Scholz, C.; Hahn, M.; Hoehne, W.
Deposited on : 2000-02-23
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

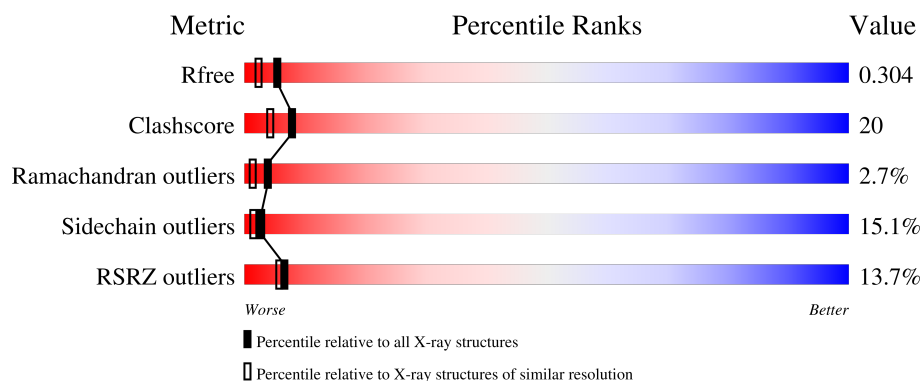
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	253	
1	B	253	
2	X	129	
2	Y	129	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5709 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 SCFV FRAGMENT 1F9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	2
			1727	1086	284	351	6			
1	B	224	Total	C	N	O	S	0	0	2
			1727	1086	284	351	6			

- Molecule 2 is a protein called TURKEY EGG-WHITE LYSOZYME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	129	Total	C	N	O	S	0	1	0
			1001	615	194	182	10			
2	Y	129	Total	C	N	O	S	0	0	0
			994	611	191	182	10			

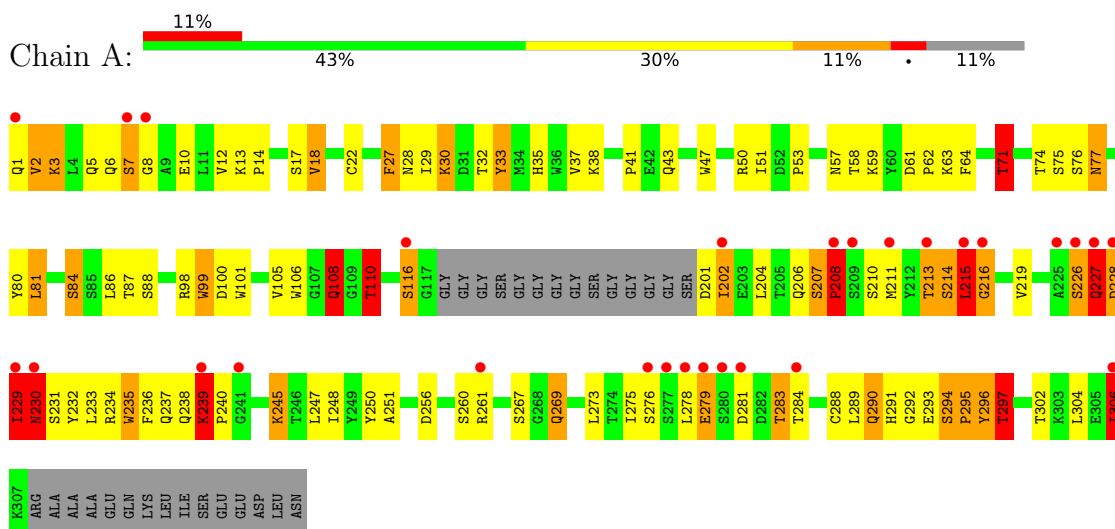
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	105	Total	O	0	0
			105	105		
3	X	53	Total	O	0	0
			53	53		
3	Y	28	Total	O	0	0
			28	28		

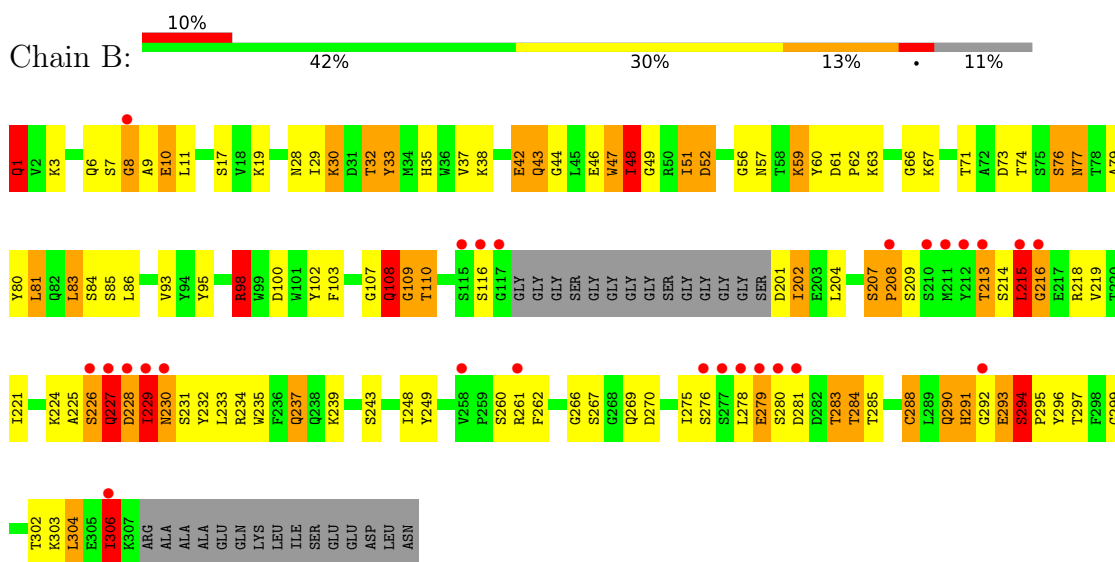
3 Residue-property plots

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 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: SCFV FRAGMENT 1F9

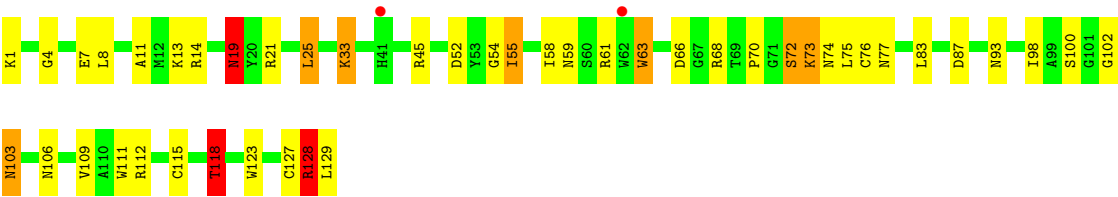


• Molecule 1: SCFV FRAGMENT 1F9

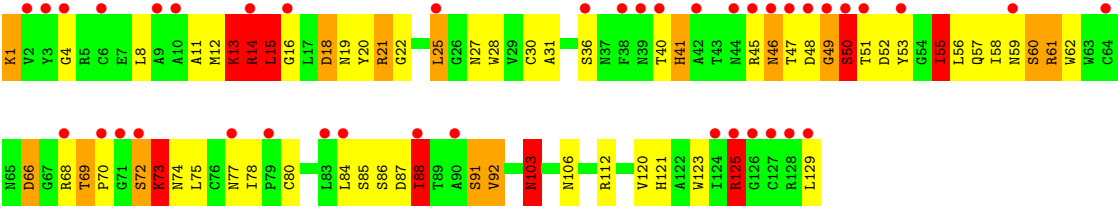


• Molecule 2: TURKEY EGG-WHITE LYSOZYME C





● Molecule 2: TURKEY EGG-WHITE LYSOZYME C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.71Å 112.44Å 80.00Å 90.00° 97.67° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.9 (20.00-2.00) 87.8 (20.00-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.306 0.227 , 0.304	Depositor DCC
R_{free} test set	2011 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5709	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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	1.45	9/1768 (0.5%)	2.42	90/2404 (3.7%)
1	B	1.52	18/1768 (1.0%)	2.39	91/2404 (3.8%)
2	X	1.54	5/1026 (0.5%)	2.15	37/1385 (2.7%)
2	Y	1.28	3/1015 (0.3%)	2.22	46/1371 (3.4%)
All	All	1.46	35/5577 (0.6%)	2.33	264/7564 (3.5%)

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	4
1	B	0	4
All	All	0	8

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	74	ASN	N-CA	8.59	1.59	1.46
1	A	294	SER	CA-C	-7.41	1.43	1.52
1	A	208	PRO	N-CA	-7.40	1.37	1.47
1	B	227	GLN	N-CA	-6.67	1.37	1.46
1	A	116	SER	C-N	-6.59	1.24	1.33
1	B	98	ARG	C-N	-6.49	1.25	1.33
1	B	47	TRP	CA-CB	-6.46	1.43	1.53
1	B	98	ARG	NE-CZ	-6.45	1.25	1.33
2	X	70	PRO	C-O	6.24	1.32	1.24
1	B	291	HIS	C-O	-6.19	1.15	1.23
1	B	267	SER	C-O	6.09	1.30	1.23
1	B	306	ILE	C-N	-6.08	1.24	1.33
1	B	47	TRP	N-CA	6.03	1.53	1.46
1	A	228	ASP	C-N	-5.99	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	TRP	CA-CB	-5.98	1.44	1.53
1	B	294	SER	CA-C	-5.97	1.45	1.52
1	A	306	ILE	C-N	-5.95	1.25	1.33
2	Y	73	LYS	C-N	-5.85	1.25	1.33
1	A	33	TYR	CA-C	5.62	1.59	1.52
2	Y	21	ARG	NE-CZ	-5.53	1.26	1.33
1	A	227	GLN	N-CA	-5.52	1.39	1.46
2	X	25	LEU	C-O	5.45	1.30	1.24
2	X	52	ASP	CA-C	5.45	1.59	1.52
1	B	66	GLY	CA-C	5.41	1.59	1.51
1	A	105	VAL	CA-C	5.39	1.59	1.52
2	X	11	ALA	N-CA	5.30	1.52	1.46
1	B	79	ALA	C-O	5.27	1.29	1.23
1	B	116	SER	C-N	-5.26	1.25	1.33
1	B	1	GLN	N-CA	5.16	1.56	1.46
1	B	10	GLU	C-N	-5.14	1.27	1.33
1	B	230	ASN	CA-CB	-5.14	1.46	1.53
1	B	8	GLY	C-N	-5.13	1.27	1.33
1	B	71	THR	C-N	-5.04	1.27	1.33
1	B	109	GLY	C-O	5.03	1.29	1.23
2	Y	88	ILE	CA-CB	5.01	1.60	1.54

All (264) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ASP	CA-CB-CG	30.66	143.26	112.60
1	A	207	SER	CA-C-O	-22.14	94.06	120.41
1	A	294	SER	CA-C-O	-20.59	91.95	120.16
2	Y	21	ARG	CD-NE-CZ	20.46	153.05	124.40
1	B	294	SER	CA-C-O	-19.56	93.36	120.16
1	B	98	ARG	CD-NE-CZ	18.43	150.20	124.40
1	B	207	SER	CA-C-O	-18.02	95.47	120.16
1	B	100	ASP	CA-CB-CG	17.23	129.83	112.60
1	A	207	SER	O-C-N	15.30	136.41	121.57
1	A	8	GLY	N-CA-C	13.62	145.45	113.18
1	A	207	SER	CA-C-N	13.56	136.79	119.84
1	A	207	SER	C-N-CA	13.56	136.79	119.84
1	B	226	SER	CA-C-N	13.40	147.13	121.54
1	B	226	SER	C-N-CA	13.40	147.13	121.54
2	Y	125	ARG	CD-NE-CZ	12.58	142.02	124.40
1	B	291	HIS	CA-C-O	12.30	135.59	121.32
1	B	227	GLN	CB-CG-CD	12.28	133.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	GLN	N-CA-CB	12.06	130.86	110.49
1	A	295	PRO	N-CA-CB	11.95	115.80	103.25
1	B	98	ARG	NE-CZ-NH1	11.95	133.45	121.50
2	X	55	ILE	CA-C-O	-11.91	107.82	120.57
2	Y	72	SER	CA-C-O	11.80	131.98	120.88
2	X	21	ARG	CD-NE-CZ	11.73	140.83	124.40
1	A	208	PRO	CA-N-CD	-11.59	95.78	112.00
2	Y	73	LYS	N-CA-C	-10.81	92.96	109.94
1	B	208	PRO	N-CA-CB	10.64	114.43	103.25
1	B	295	PRO	N-CA-CB	10.35	114.12	103.25
2	Y	46	ASN	CA-CB-CG	10.34	122.94	112.60
2	Y	112	ARG	CD-NE-CZ	10.28	138.78	124.40
2	X	55	ILE	O-C-N	10.13	132.10	121.87
1	A	214	SER	CA-C-N	10.11	140.86	121.54
1	A	214	SER	C-N-CA	10.11	140.86	121.54
1	B	48	ILE	CA-CB-CG2	9.51	126.67	110.50
1	B	230	ASN	N-CA-C	-9.50	93.94	108.67
1	B	208	PRO	CA-N-CD	-9.34	98.92	112.00
1	A	208	PRO	N-CA-CB	9.34	113.05	103.25
2	X	68	ARG	CD-NE-CZ	9.30	137.42	124.40
1	A	214	SER	CA-C-O	9.26	130.70	120.70
2	X	73	LYS	CA-C-N	-9.26	110.43	123.20
2	X	73	LYS	C-N-CA	-9.26	110.43	123.20
1	A	295	PRO	CA-N-CD	-9.18	99.14	112.00
1	A	99	TRP	CA-CB-CG	9.13	130.95	113.60
2	Y	13	LYS	CA-C-O	-9.13	111.59	121.99
1	B	231	SER	N-CA-C	9.10	123.91	111.90
1	B	42	GLU	CA-CB-CG	9.08	132.26	114.10
1	A	226	SER	CA-C-N	9.05	138.83	121.54
1	A	226	SER	C-N-CA	9.05	138.83	121.54
1	A	99	TRP	N-CA-CB	8.95	124.62	110.57
1	B	295	PRO	N-CD-CG	8.89	116.53	103.20
1	B	295	PRO	CA-N-CD	-8.89	99.56	112.00
1	A	295	PRO	N-CD-CG	8.82	116.43	103.20
1	B	281	ASP	CA-CB-CG	8.81	121.41	112.60
1	A	229	ILE	N-CA-CB	8.80	125.76	111.23
1	B	8	GLY	CA-C-N	8.76	137.89	121.69
1	B	8	GLY	C-N-CA	8.76	137.89	121.69
1	B	8	GLY	O-C-N	-8.71	111.38	122.70
1	B	208	PRO	N-CD-CG	8.65	116.17	103.20
1	A	61	ASP	N-CA-C	-8.62	96.66	109.42
1	A	110	THR	CA-C-O	8.58	130.67	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	LYS	CA-CB-CG	8.39	130.88	114.10
1	A	256	ASP	CA-CB-CG	-8.36	104.24	112.60
1	B	231	SER	N-CA-CB	-8.28	99.58	112.08
1	A	239	LYS	CA-CB-CG	8.24	130.58	114.10
2	Y	61	ARG	CD-NE-CZ	8.21	135.89	124.40
1	B	207	SER	CA-C-N	8.19	130.08	119.84
1	B	207	SER	C-N-CA	8.19	130.08	119.84
2	X	55	ILE	N-CA-CB	8.16	124.61	110.65
2	X	55	ILE	CB-CA-C	-8.15	99.52	112.16
1	B	61	ASP	N-CA-C	-8.08	99.47	109.65
2	Y	47	THR	CA-C-N	8.05	133.82	120.70
2	Y	47	THR	C-N-CA	8.05	133.82	120.70
1	B	9	ALA	CA-C-O	-7.89	111.12	120.43
2	X	70	PRO	N-CA-C	7.82	125.40	113.75
1	A	260	SER	CA-C-N	7.74	131.69	120.38
1	A	260	SER	C-N-CA	7.74	131.69	120.38
2	X	118	THR	N-CA-CB	-7.66	99.48	110.44
1	A	228	ASP	CA-C-N	7.63	135.71	121.97
1	A	228	ASP	C-N-CA	7.63	135.71	121.97
1	A	57	ASN	CA-CB-CG	7.52	120.12	112.60
1	B	229	ILE	CA-C-O	-7.49	111.42	120.78
2	X	106	ASN	CA-CB-CG	-7.49	105.11	112.60
1	B	237	GLN	OE1-CD-NE2	7.37	129.97	122.60
2	Y	66	ASP	CA-CB-CG	7.36	119.96	112.60
2	X	45	ARG	CD-NE-CZ	7.35	134.69	124.40
2	Y	48	ASP	CA-C-O	7.32	126.57	118.52
2	Y	48	ASP	N-CA-C	-7.26	103.41	114.16
1	B	229	ILE	CA-C-N	-7.25	111.19	121.99
1	B	229	ILE	C-N-CA	-7.25	111.19	121.99
2	X	72	SER	CA-C-O	7.24	129.27	121.16
2	Y	49	GLY	N-CA-C	-7.23	96.04	113.18
1	A	2	VAL	CA-C-O	-7.21	112.63	120.85
1	B	47	TRP	CA-C-N	-7.19	113.86	122.35
1	B	47	TRP	C-N-CA	-7.19	113.86	122.35
2	Y	4	GLY	N-CA-C	-7.16	101.65	112.60
1	B	226	SER	O-C-N	-7.14	111.61	122.61
2	Y	87	ASP	CA-C-N	7.13	132.33	120.64
2	Y	87	ASP	C-N-CA	7.13	132.33	120.64
1	B	48	ILE	CB-CG1-CD1	-7.12	98.84	113.80
2	X	73	LYS	N-CA-C	-7.05	98.44	109.72
1	B	234	ARG	CA-CB-CG	7.05	128.19	114.10
1	B	48	ILE	N-CA-C	-6.95	105.83	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	GLN	CB-CG-CD	6.84	124.22	112.60
2	X	74	ASN	CB-CA-C	6.79	121.75	111.70
2	Y	106	ASN	CA-CB-CG	-6.78	105.82	112.60
2	Y	86	SER	CA-C-O	6.77	126.59	119.14
1	B	33	TYR	CA-C-O	-6.75	113.41	120.70
2	Y	86	SER	N-CA-C	-6.74	105.21	113.50
1	A	71	THR	N-CA-CB	-6.72	99.99	111.69
1	A	98	ARG	CD-NE-CZ	6.67	133.74	124.40
1	B	37	VAL	O-C-N	-6.64	116.03	123.20
1	A	267	SER	CA-C-O	-6.61	114.37	121.38
1	B	52	ASP	CA-CB-CG	6.58	119.18	112.60
2	Y	13	LYS	N-CA-C	-6.57	102.32	110.41
1	A	228	ASP	O-C-N	-6.55	113.88	122.59
1	A	229	ILE	CA-C-N	-6.55	112.22	121.72
1	A	229	ILE	C-N-CA	-6.55	112.22	121.72
2	X	77	ASN	OD1-CG-ND2	-6.54	116.06	122.60
1	B	207	SER	O-C-N	6.51	128.81	121.32
2	X	8	LEU	CA-C-O	6.49	127.30	120.42
1	A	214	SER	O-C-N	-6.49	114.79	123.23
1	A	110	THR	CA-CB-CG2	6.49	121.53	110.50
1	A	37	VAL	O-C-N	6.46	130.02	123.10
2	X	63	TRP	N-CA-C	6.42	121.24	113.41
1	B	227	GLN	OE1-CD-NE2	-6.39	116.21	122.60
2	X	45	ARG	NE-CZ-NH1	6.39	127.89	121.50
1	A	201	ASP	N-CA-CB	6.36	121.32	110.50
1	A	8	GLY	O-C-N	-6.34	114.46	122.70
2	X	66	ASP	CA-CB-CG	6.33	118.94	112.60
2	X	19	ASN	CA-CB-CG	-6.29	106.31	112.60
1	A	231	SER	N-CA-C	6.29	124.19	110.80
1	B	234	ARG	CD-NE-CZ	6.26	133.16	124.40
1	A	27	PHE	CA-CB-CG	6.25	120.06	113.80
1	B	9	ALA	N-CA-C	-6.25	98.42	108.55
1	B	229	ILE	N-CA-CB	-6.22	100.97	111.23
1	A	3	LYS	N-CA-C	6.13	118.17	108.79
1	B	218	ARG	CA-C-N	-6.13	115.11	123.14
1	B	218	ARG	C-N-CA	-6.13	115.11	123.14
1	A	226	SER	O-C-N	-6.12	114.45	122.59
2	Y	48	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	202	ILE	N-CA-CB	6.08	117.16	110.53
1	B	266	GLY	CA-C-N	6.07	132.18	122.10
1	B	266	GLY	C-N-CA	6.07	132.18	122.10
1	B	9	ALA	N-CA-CB	6.05	121.69	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ILE	N-CA-C	6.00	116.80	109.30
1	B	62	PRO	CA-C-N	5.97	128.60	120.54
1	B	62	PRO	C-N-CA	5.97	128.60	120.54
2	Y	92	VAL	CB-CA-C	-5.97	104.20	112.02
1	A	227	GLN	CB-CG-CD	5.96	122.74	112.60
1	B	243	SER	CA-CB-OG	-5.96	99.18	111.10
1	A	297	THR	N-CA-CB	-5.96	100.53	111.37
1	B	98	ARG	NH1-CZ-NH2	-5.95	111.56	119.30
1	A	61	ASP	N-CA-CB	5.94	119.17	109.90
2	X	106	ASN	N-CA-C	5.93	119.61	112.38
1	A	234	ARG	CG-CD-NE	5.93	125.04	112.00
1	A	235	TRP	CA-C-O	-5.92	113.93	120.38
2	X	87	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	108	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	A	239	LYS	N-CA-CB	5.90	118.26	109.88
1	A	14	PRO	CA-C-O	-5.88	114.72	121.36
1	A	230	ASN	N-CA-CB	5.86	119.42	109.87
1	B	229	ILE	N-CA-C	-5.86	97.15	109.34
1	A	231	SER	N-CA-CB	-5.85	100.61	110.49
1	B	230	ASN	N-CA-CB	5.83	119.27	109.94
2	Y	123	TRP	N-CA-C	5.81	119.84	112.87
2	Y	14	ARG	CA-C-O	-5.79	112.23	120.51
1	A	81	LEU	CB-CG-CD2	5.78	128.04	110.70
1	A	234	ARG	CD-NE-CZ	5.78	132.49	124.40
2	Y	123	TRP	CA-CB-CG	-5.75	102.67	113.60
2	X	106	ASN	OD1-CG-ND2	5.75	128.34	122.60
1	A	64	PHE	CA-CB-CG	-5.74	108.06	113.80
2	Y	14	ARG	N-CA-C	-5.74	98.57	110.80
1	B	260	SER	CA-C-N	5.73	129.77	120.60
1	B	260	SER	C-N-CA	5.73	129.77	120.60
1	A	17	SER	CA-CB-OG	-5.71	99.67	111.10
1	A	275	ILE	CA-C-O	-5.70	114.46	120.39
1	B	76	SER	CA-C-N	5.70	130.22	122.19
1	B	76	SER	C-N-CA	5.70	130.22	122.19
2	Y	74	ASN	N-CA-C	-5.69	98.69	110.80
1	B	61	ASP	CA-C-N	5.65	125.49	119.28
1	B	61	ASP	C-N-CA	5.65	125.49	119.28
1	B	76	SER	CA-C-O	5.64	126.32	119.11
1	A	202	ILE	CA-C-N	5.63	130.26	122.77
1	A	202	ILE	C-N-CA	5.63	130.26	122.77
2	X	25	LEU	O-C-N	-5.62	116.16	122.12
2	Y	91	SER	CA-C-N	5.62	127.75	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	91	SER	C-N-CA	5.62	127.75	120.56
1	A	236	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	71	THR	O-C-N	-5.60	116.40	123.17
2	X	93	ASN	CA-C-O	-5.59	113.78	120.10
1	B	293	GLU	CA-CB-CG	5.58	125.27	114.10
1	B	60	TYR	CB-CA-C	-5.58	98.35	109.79
1	A	3	LYS	CA-CB-CG	5.58	125.26	114.10
1	A	245	LYS	CA-C-O	-5.55	114.89	121.16
2	X	25	LEU	CA-C-O	5.52	126.59	120.63
1	A	281	ASP	N-CA-CB	-5.51	101.14	110.41
1	A	269	GLN	CA-CB-CG	5.51	125.12	114.10
1	B	46	GLU	CA-C-N	-5.50	113.63	121.50
1	B	46	GLU	C-N-CA	-5.50	113.63	121.50
1	A	99	TRP	O-C-N	5.50	129.78	123.29
1	A	296	TYR	CA-C-N	-5.50	114.05	122.62
1	A	296	TYR	C-N-CA	-5.50	114.05	122.62
1	A	58	THR	CA-C-O	-5.48	115.03	121.44
1	A	228	ASP	CA-CB-CG	5.47	118.07	112.60
2	X	74	ASN	N-CA-C	-5.46	100.85	108.54
1	B	32	THR	CA-CB-OG1	-5.44	101.44	109.60
2	Y	103	ASN	CA-C-O	5.43	126.08	119.78
1	B	38	LYS	CA-C-O	-5.42	114.89	121.28
1	A	229	ILE	CA-C-O	-5.41	114.02	120.78
1	B	288	CYS	N-CA-CB	5.41	119.00	110.56
2	Y	88	ILE	N-CA-C	5.41	120.01	112.50
1	A	226	SER	CA-C-O	5.40	128.24	120.51
1	B	262	PHE	CA-CB-CG	5.40	119.20	113.80
1	B	8	GLY	N-CA-C	5.40	125.98	113.18
2	Y	50	SER	N-CA-CB	-5.38	101.39	110.49
1	B	275	ILE	CA-C-O	-5.38	114.77	120.53
1	A	33	TYR	N-CA-C	-5.37	100.95	109.76
2	X	7	GLU	CA-CB-CG	5.37	124.84	114.10
1	A	7	SER	CA-C-O	-5.36	114.59	120.70
1	B	93	VAL	CA-C-O	-5.36	114.83	120.57
2	Y	55	ILE	CA-C-N	-5.34	114.13	122.73
2	Y	55	ILE	C-N-CA	-5.34	114.13	122.73
2	Y	18	ASP	CA-CB-CG	-5.33	107.27	112.60
2	X	4	GLY	N-CA-C	-5.31	104.93	112.37
1	A	38	LYS	CA-C-O	-5.30	115.09	120.71
2	X	11	ALA	N-CA-CB	-5.30	102.33	110.12
1	A	22	CYS	N-CA-CB	-5.29	102.16	110.79
1	B	284	THR	CB-CA-C	-5.29	99.90	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	SER	N-CA-CB	-5.28	102.40	110.85
1	B	299	GLY	N-CA-C	-5.27	105.79	112.54
2	Y	4	GLY	CA-C-O	-5.26	115.10	122.36
2	Y	77	ASN	CA-CB-CG	-5.26	107.34	112.60
1	B	215	LEU	O-C-N	-5.24	115.62	122.59
1	B	207	SER	N-CA-C	5.23	121.37	109.81
2	X	127	CYS	CA-C-O	-5.23	115.16	120.71
2	Y	28	TRP	CA-C-O	-5.22	114.88	120.42
1	A	62	PRO	CA-C-N	5.22	128.95	120.60
1	A	62	PRO	C-N-CA	5.22	128.95	120.60
2	Y	88	ILE	CA-C-O	5.21	125.89	119.58
1	B	110	THR	CA-CB-CG2	5.21	119.35	110.50
1	B	110	THR	N-CA-CB	5.20	119.80	110.80
2	Y	36	SER	N-CA-C	5.17	120.98	114.31
2	X	54	GLY	N-CA-C	5.17	123.30	112.45
2	Y	15	LEU	N-CA-C	5.16	121.78	110.80
2	X	128	ARG	CA-C-O	-5.16	113.14	120.51
2	Y	13	LYS	CA-CB-CG	5.15	124.40	114.10
1	A	18	VAL	N-CA-CB	5.15	121.55	111.92
2	X	74	ASN	OD1-CG-ND2	5.13	127.73	122.60
1	A	206	GLN	CB-CG-CD	5.12	121.30	112.60
1	A	57	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	302	THR	CA-CB-OG1	5.11	117.26	109.60
1	B	215	LEU	N-CA-C	5.10	121.66	110.80
1	B	234	ARG	CA-C-N	5.09	129.75	122.72
1	B	234	ARG	C-N-CA	5.09	129.75	122.72
2	X	13	LYS	CA-C-O	5.08	125.81	120.42
1	A	99	TRP	CB-CA-C	-5.08	100.93	109.72
1	A	207	SER	CB-CA-C	5.08	116.51	108.84
1	B	46	GLU	CA-C-O	-5.06	114.89	120.36
2	X	33	LYS	CA-C-O	-5.06	115.50	120.82
1	B	10	GLU	CB-CG-CD	5.06	121.20	112.60
2	Y	69	THR	CB-CA-C	5.06	116.62	109.08
1	A	105	VAL	CB-CA-C	-5.05	101.95	111.30
1	B	281	ASP	CB-CA-C	-5.03	99.94	109.95
2	Y	55	ILE	CB-CA-C	-5.02	105.36	112.14
2	Y	22	GLY	N-CA-C	5.02	122.04	115.47

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	SER	Peptide,Mainchain
1	A	294	SER	Peptide,Mainchain
1	B	207	SER	Peptide,Mainchain
1	B	294	SER	Peptide,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	1727	0	1648	74	0
1	B	1727	0	1648	90	0
2	X	1001	0	965	21	0
2	Y	994	0	956	37	0
3	A	74	0	0	6	0
3	B	105	0	0	4	0
3	X	53	0	0	3	0
3	Y	28	0	0	0	0
All	All	5709	0	5217	211	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (211) 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:30:LYS:HE3	1:A:74:THR:HB	1.43	1.01
1:A:71:THR:HG22	1:A:80:TYR:HB2	1.42	0.99
1:A:278:LEU:HD21	1:A:306:ILE:HD12	1.47	0.96
1:A:35:HIS:HD2	1:A:47:TRP:HE1	1.10	0.95
1:B:29:ILE:H	1:B:77:ASN:HD21	1.11	0.94
1:B:43:GLN:HE21	1:B:44:GLY:H	1.15	0.94
1:B:229:ILE:HG21	1:B:232:TYR:HB2	1.49	0.92
1:B:229:ILE:HG12	1:B:232:TYR:HD2	1.34	0.91
1:B:35:HIS:HD2	1:B:47:TRP:HE1	1.14	0.90
1:B:6:GLN:H	1:B:108:GLN:HE22	1.19	0.89
1:B:29:ILE:H	1:B:77:ASN:ND2	1.71	0.88
1:B:1:GLN:HE22	1:B:3:LYS:HE3	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HE21	1:A:108:GLN:H	1.23	0.87
2:Y:13:LYS:O	2:Y:14:ARG:HB3	1.75	0.86
1:B:229:ILE:HG12	1:B:232:TYR:CD2	2.10	0.86
1:B:83:LEU:HB3	1:B:86:LEU:HD21	1.56	0.85
1:A:233:LEU:HD11	1:A:288:CYS:HB2	1.60	0.84
1:B:229:ILE:CG2	1:B:232:TYR:H	1.90	0.83
1:B:290:GLN:NE2	1:B:292:GLY:H	1.78	0.81
1:A:6:GLN:H	1:A:108:GLN:HE22	1.28	0.80
1:A:261:ARG:HH11	1:A:279:GLU:HG2	1.48	0.78
1:A:290:GLN:NE2	1:A:292:GLY:H	1.81	0.77
1:A:290:GLN:HG3	1:A:297:THR:HG22	1.64	0.77
1:A:35:HIS:CD2	1:A:47:TRP:HE1	2.01	0.76
1:B:43:GLN:NE2	1:B:44:GLY:H	1.85	0.75
1:B:290:GLN:HG3	1:B:297:THR:HG22	1.69	0.75
1:A:290:GLN:HE22	1:A:293:GLU:H	1.35	0.75
2:Y:8:LEU:HG	2:Y:12:MET:HE3	1.67	0.74
1:B:228:ASP:O	1:B:229:ILE:HB	1.87	0.74
1:B:229:ILE:HG23	1:B:232:TYR:H	1.51	0.74
2:Y:1:LYS:HD3	2:Y:41:HIS:ND1	2.02	0.74
1:B:35:HIS:CD2	1:B:47:TRP:HE1	2.04	0.73
1:B:290:GLN:HE22	1:B:293:GLU:H	1.37	0.71
1:A:87:THR:CG2	1:B:67:LYS:HG3	2.20	0.70
1:B:227:GLN:HB2	3:B:2095:HOH:O	1.89	0.70
1:B:29:ILE:N	1:B:77:ASN:HD21	1.86	0.70
1:B:81:LEU:HD12	1:B:83:LEU:HD22	1.72	0.69
1:A:215:LEU:CD1	1:A:215:LEU:H	2.05	0.69
1:A:2:VAL:HG13	3:A:2009:HOH:O	1.92	0.69
2:X:63:TRP:O	2:X:76:CYS:HB2	1.95	0.67
1:A:239:LYS:HA	1:A:284:THR:HG22	1.75	0.67
1:B:229:ILE:HG21	1:B:232:TYR:CB	2.24	0.67
1:B:98:ARG:O	1:B:98:ARG:HG3	1.95	0.66
1:A:29:ILE:H	1:A:77:ASN:HD21	1.41	0.66
1:A:30:LYS:H	1:A:30:LYS:NZ	1.93	0.65
2:Y:59:ASN:ND2	2:Y:61:ARG:HB3	2.12	0.65
1:A:87:THR:HG21	1:B:67:LYS:HG3	1.78	0.65
2:Y:50:SER:HB2	2:Y:60:SER:OG	1.97	0.65
1:A:33:TYR:H	2:X:103:ASN:ND2	1.94	0.65
1:A:261:ARG:NH1	1:A:279:GLU:HG2	2.11	0.65
1:A:290:GLN:CG	1:A:297:THR:HG22	2.28	0.63
2:Y:61:ARG:O	2:Y:72:SER:HA	1.98	0.63
1:A:230:ASN:HB2	3:A:2065:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LYS:H	1:B:30:LYS:CD	2.13	0.62
1:A:290:GLN:HE21	1:A:292:GLY:H	1.45	0.62
1:B:290:GLN:HE21	1:B:292:GLY:H	1.45	0.62
1:A:237:GLN:HB2	1:A:247:LEU:HD11	1.81	0.62
2:Y:50:SER:HB3	2:Y:69:THR:HG21	1.81	0.61
1:A:18:VAL:HG22	1:A:86:LEU:HD11	1.82	0.61
1:B:30:LYS:HE2	3:B:2050:HOH:O	2.00	0.61
2:X:25:LEU:HD23	2:X:129:LEU:HD21	1.82	0.61
1:A:227:GLN:H	1:A:269:GLN:HG2	1.65	0.61
1:B:290:GLN:CG	1:B:297:THR:HG22	2.31	0.60
2:Y:50:SER:HB3	2:Y:69:THR:CG2	2.31	0.60
1:A:30:LYS:H	1:A:30:LYS:HZ2	1.47	0.60
1:B:30:LYS:HD2	1:B:74:THR:HB	1.83	0.59
1:B:1:GLN:NE2	1:B:3:LYS:HE3	2.13	0.59
1:B:219:VAL:HG11	1:B:304:LEU:HD11	1.85	0.59
1:A:202:ILE:O	1:A:297:THR:HG21	2.04	0.58
1:B:28:ASN:HB3	1:B:30:LYS:HG2	1.84	0.58
2:Y:20:TYR:CE1	2:Y:21:ARG:HG2	2.39	0.58
1:B:6:GLN:N	1:B:108:GLN:HE22	1.98	0.58
1:B:6:GLN:HB3	1:B:110:THR:CG2	2.33	0.58
1:B:227:GLN:H	1:B:269:GLN:HG2	1.68	0.58
2:X:14[B]:ARG:NH2	3:X:2009:HOH:O	2.26	0.57
1:A:84:SER:HB3	1:B:85:SER:OG	2.04	0.57
2:Y:60:SER:HB2	2:Y:80:CYS:SG	2.45	0.57
2:Y:121:HIS:CE1	2:Y:125:ARG:HH11	2.22	0.57
1:B:6:GLN:HB3	1:B:110:THR:HG23	1.86	0.56
2:X:115:CYS:O	2:X:118:THR:HB	2.05	0.56
1:B:221:ILE:HG12	1:B:302:THR:HG21	1.87	0.56
1:A:229:ILE:HG13	1:A:230:ASN:H	1.71	0.56
1:B:7:SER:O	1:B:110:THR:HG22	2.07	0.55
2:Y:59:ASN:HD21	2:Y:61:ARG:HB3	1.69	0.55
1:A:29:ILE:H	1:A:77:ASN:ND2	2.04	0.55
1:B:233:LEU:HD11	1:B:288:CYS:HB2	1.87	0.54
1:B:261:ARG:HH11	1:B:279:GLU:HG2	1.72	0.54
1:B:290:GLN:NE2	1:B:292:GLY:N	2.54	0.54
2:Y:18:ASP:HB2	2:Y:25:LEU:HD23	1.89	0.54
1:B:227:GLN:HA	1:B:269:GLN:HG3	1.89	0.54
1:B:48:ILE:HG13	1:B:49:GLY:N	2.23	0.53
1:B:81:LEU:HD12	1:B:83:LEU:CD2	2.37	0.53
2:Y:61:ARG:HA	2:Y:69:THR:HG21	1.91	0.53
1:A:99:TRP:CH2	1:A:106:TRP:CZ2	2.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:H	1:A:215:LEU:HD12	1.73	0.52
1:A:283:THR:O	1:A:284:THR:HG23	2.09	0.52
1:B:30:LYS:H	1:B:30:LYS:HD3	1.75	0.52
1:A:208:PRO:HG2	1:A:211:MET:HE2	1.91	0.51
2:X:59:ASN:ND2	2:X:61:ARG:H	2.07	0.51
1:A:6:GLN:HB3	1:A:110:THR:HG22	1.92	0.51
1:A:6:GLN:H	1:A:108:GLN:NE2	2.01	0.51
1:B:33:TYR:H	2:Y:103:ASN:ND2	2.08	0.51
1:B:59:LYS:HG3	3:B:2102:HOH:O	2.11	0.51
1:B:81:LEU:HD11	1:B:83:LEU:HD13	1.93	0.51
1:B:204:LEU:HG	1:B:297:THR:HG23	1.94	0.50
1:A:27:PHE:CE1	1:A:32:THR:HG21	2.47	0.50
2:Y:11:ALA:HB1	2:Y:88:ILE:HD13	1.93	0.49
2:Y:15:LEU:HD13	2:Y:92:VAL:HG21	1.94	0.49
1:A:30:LYS:CE	1:A:74:THR:HB	2.29	0.49
1:A:28:ASN:HB3	1:A:30:LYS:NZ	2.27	0.49
1:A:214:SER:O	1:A:216:GLY:N	2.42	0.49
2:X:61:ARG:HH11	2:X:61:ARG:HG3	1.77	0.49
1:A:35:HIS:HE1	2:X:102:GLY:O	1.95	0.49
2:X:111:TRP:CD1	2:X:115:CYS:HB2	2.47	0.49
1:A:261:ARG:HD2	1:A:279:GLU:CD	2.38	0.49
1:A:204:LEU:HG	1:A:297:THR:HG23	1.94	0.49
1:B:28:ASN:HB3	1:B:30:LYS:CG	2.42	0.49
2:X:61:ARG:HD2	3:X:2029:HOH:O	2.11	0.49
1:A:290:GLN:NE2	1:A:292:GLY:N	2.56	0.48
1:A:229:ILE:HG13	1:A:230:ASN:N	2.28	0.48
1:A:30:LYS:HE3	1:A:74:THR:CB	2.30	0.48
1:B:48:ILE:HD11	1:B:81:LEU:HD21	1.95	0.48
1:B:204:LEU:CD2	1:B:225:ALA:HB2	2.44	0.48
1:B:103:PHE:HE2	2:Y:62:TRP:HH2	1.60	0.48
1:B:229:ILE:HD13	1:B:292:GLY:O	2.13	0.48
2:Y:45:ARG:HD3	2:Y:68:ARG:HH12	1.79	0.48
1:B:73:ASP:CG	1:B:76:SER:HB3	2.39	0.48
1:B:261:ARG:HD2	1:B:279:GLU:OE2	2.14	0.47
1:B:290:GLN:HG3	1:B:297:THR:CG2	2.41	0.47
2:Y:66:ASP:HB3	2:Y:80:CYS:SG	2.54	0.47
1:A:238:GLN:O	1:A:284:THR:HB	2.14	0.47
2:X:33:LYS:HG2	2:X:123:TRP:CH2	2.49	0.47
1:A:33:TYR:H	2:X:103:ASN:HD21	1.59	0.47
1:A:239:LYS:HB3	1:A:240:PRO:HD2	1.95	0.47
2:Y:15:LEU:CD1	2:Y:88:ILE:HG12	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:14:ARG:O	2:Y:16:GLY:N	2.48	0.47
1:B:215:LEU:HD13	1:B:280:SER:HB2	1.97	0.47
1:A:219:VAL:HG21	1:A:278:LEU:HD13	1.97	0.47
1:B:284:THR:HB	1:B:285:THR:H	1.65	0.47
2:Y:27:ASN:ND2	2:Y:120:VAL:HG21	2.29	0.47
1:A:227:GLN:NE2	1:A:229:ILE:H	2.13	0.46
2:Y:73:LYS:HD2	2:Y:73:LYS:N	2.30	0.46
1:B:6:GLN:HE21	1:B:107:GLY:HA3	1.80	0.46
1:B:209:SER:HB2	3:B:2071:HOH:O	2.16	0.46
1:B:214:SER:O	1:B:216:GLY:N	2.42	0.46
2:X:109:VAL:O	2:X:112:ARG:HB2	2.15	0.46
1:B:237:GLN:HG2	1:B:284:THR:HG21	1.98	0.46
1:B:19:LYS:HE2	1:B:80:TYR:CD2	2.51	0.46
1:B:227:GLN:O	1:B:228:ASP:C	2.58	0.46
1:B:6:GLN:NE2	1:B:109:GLY:H	2.14	0.45
1:A:35:HIS:CD2	1:A:50:ARG:HB3	2.52	0.45
2:X:25:LEU:CD2	2:X:129:LEU:HD21	2.47	0.45
1:B:81:LEU:CD1	1:B:83:LEU:HD13	2.46	0.45
1:A:27:PHE:HD2	3:A:2009:HOH:O	2.00	0.45
2:X:61:ARG:O	2:X:72:SER:HA	2.15	0.45
1:B:98:ARG:HH11	1:B:103:PHE:HB3	1.81	0.45
1:A:289:LEU:HD11	1:A:296:TYR:HB3	1.97	0.45
2:X:14[B]:ARG:NH1	3:X:2009:HOH:O	2.50	0.45
2:Y:56:LEU:HB2	2:Y:58:ILE:HD11	1.99	0.45
1:A:295:PRO:HD2	3:A:2070:HOH:O	2.16	0.45
1:B:235:TRP:HB2	1:B:248:ILE:HB	1.99	0.45
2:Y:59:ASN:ND2	2:Y:61:ARG:H	2.14	0.44
1:A:99:TRP:HH2	1:A:106:TRP:CZ2	2.34	0.44
1:B:51:ILE:HD12	1:B:52:ASP:N	2.32	0.44
1:B:59:LYS:HD2	1:B:59:LYS:HA	1.62	0.44
1:B:213:THR:HG21	1:B:219:VAL:HG21	1.98	0.44
1:B:261:ARG:NH1	1:B:279:GLU:HG2	2.33	0.44
1:B:32:THR:HB	2:Y:103:ASN:HD21	1.81	0.44
2:Y:88:ILE:HG13	2:Y:92:VAL:HG23	1.99	0.44
1:A:27:PHE:HE1	1:A:32:THR:HG21	1.82	0.43
2:Y:56:LEU:O	2:Y:57:GLN:C	2.60	0.43
1:A:227:GLN:HA	1:A:269:GLN:HG3	1.99	0.43
1:B:108:GLN:NE2	1:B:108:GLN:H	2.17	0.43
1:B:28:ASN:HA	1:B:77:ASN:HD21	1.82	0.43
2:Y:55:ILE:H	2:Y:55:ILE:HG13	1.45	0.43
2:Y:40:THR:O	2:Y:84:LEU:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:NZ	1:A:5:GLN:HB2	2.33	0.43
1:B:33:TYR:H	2:Y:103:ASN:HD21	1.65	0.43
1:B:102:TYR:HA	1:B:249:TYR:CE2	2.53	0.43
1:B:202:ILE:O	1:B:297:THR:HG21	2.18	0.43
2:Y:51:THR:HB	2:Y:53:TYR:CE2	2.53	0.43
1:A:208:PRO:HG2	1:A:211:MET:CE	2.49	0.43
1:B:204:LEU:HD23	1:B:225:ALA:HB2	2.00	0.43
2:X:58:ILE:HB	2:X:83:LEU:HD13	2.01	0.43
1:B:51:ILE:HD13	1:B:57:ASN:O	2.19	0.42
1:B:227:GLN:HA	1:B:269:GLN:CG	2.48	0.42
1:A:239:LYS:CA	1:A:284:THR:HG22	2.44	0.42
1:A:12:VAL:HG11	1:A:18:VAL:CG1	2.49	0.42
1:B:6:GLN:HE22	1:B:95:TYR:HA	1.85	0.42
1:A:229:ILE:HG23	1:A:232:TYR:CD2	2.54	0.42
1:B:228:ASP:O	1:B:229:ILE:CB	2.48	0.42
2:X:19:ASN:HD22	2:X:19:ASN:HA	1.69	0.42
1:A:51:ILE:O	1:A:53:PRO:HD3	2.20	0.42
1:A:213:THR:OG1	1:A:278:LEU:HD22	2.20	0.42
2:Y:49:GLY:O	2:Y:50:SER:C	2.63	0.42
1:A:100:ASP:O	1:A:101:TRP:C	2.61	0.42
1:B:283:THR:O	1:B:284:THR:HG23	2.19	0.42
1:B:291:HIS:HA	1:B:296:TYR:CD1	2.54	0.42
2:X:63:TRP:CE2	2:X:98:ILE:HG12	2.54	0.42
2:Y:30:CYS:O	2:Y:31:ALA:C	2.63	0.42
1:A:250:TYR:O	1:A:251:ALA:HB3	2.20	0.41
1:A:239:LYS:HG3	1:A:284:THR:CG2	2.50	0.41
1:B:51:ILE:HD11	1:B:56:GLY:HA2	2.02	0.41
1:A:291:HIS:HE1	3:A:2064:HOH:O	2.03	0.41
2:Y:69:THR:HA	2:Y:70:PRO:HD3	1.77	0.41
1:A:291:HIS:HD2	2:X:100:SER:O	2.03	0.41
1:B:224:LYS:HG2	1:B:270:ASP:OD1	2.22	0.40
1:A:71:THR:HB	3:A:2030:HOH:O	2.21	0.40
2:X:59:ASN:ND2	2:X:61:ARG:HB3	2.36	0.40
2:Y:52:ASP:HB3	2:Y:57:GLN:HB3	2.02	0.40
1:A:235:TRP:HB2	1:A:248:ILE:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/253 (87%)	200 (91%)	13 (6%)	7 (3%)	3	1
1	B	220/253 (87%)	202 (92%)	10 (4%)	8 (4%)	2	1
2	X	128/129 (99%)	123 (96%)	4 (3%)	1 (1%)	16	11
2	Y	127/129 (98%)	106 (84%)	18 (14%)	3 (2%)	4	2
All	All	695/764 (91%)	631 (91%)	45 (6%)	19 (3%)	4	1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	LEU
1	A	229	ILE
1	A	276	SER
1	B	8	GLY
1	B	215	LEU
1	B	228	ASP
1	B	229	ILE
2	Y	15	LEU
2	Y	50	SER
1	A	227	GLN
1	A	228	ASP
1	B	276	SER
2	Y	14	ARG
1	B	216	GLY
2	X	128	ARG
1	A	208	PRO
1	B	208	PRO
1	A	216	GLY
1	B	306	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	191/207 (92%)	158 (83%)	33 (17%)	2	1
1	B	191/207 (92%)	161 (84%)	30 (16%)	2	1
2	X	104/103 (101%)	96 (92%)	8 (8%)	12	8
2	Y	103/103 (100%)	85 (82%)	18 (18%)	2	1
All	All	589/620 (95%)	500 (85%)	89 (15%)	3	1

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	7	SER
1	A	10	GLU
1	A	13	LYS
1	A	30	LYS
1	A	41	PRO
1	A	43	GLN
1	A	59	LYS
1	A	63	LYS
1	A	71	THR
1	A	75	SER
1	A	76	SER
1	A	77	ASN
1	A	81	LEU
1	A	88	SER
1	A	108	GLN
1	A	110	THR
1	A	116	SER
1	A	210	SER
1	A	213	THR
1	A	215	LEU
1	A	226	SER
1	A	227	GLN
1	A	230	ASN

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Mol	Chain	Res	Type
1	A	239	LYS
1	A	245	LYS
1	A	273	LEU
1	A	279	GLU
1	A	283	THR
1	A	290	GLN
1	A	297	THR
1	A	304	LEU
1	A	306	ILE
1	B	1	GLN
1	B	10	GLU
1	B	11	LEU
1	B	17	SER
1	B	30	LYS
1	B	42	GLU
1	B	43	GLN
1	B	48	ILE
1	B	51	ILE
1	B	59	LYS
1	B	77	ASN
1	B	81	LEU
1	B	83	LEU
1	B	84	SER
1	B	98	ARG
1	B	108	GLN
1	B	201	ASP
1	B	213	THR
1	B	226	SER
1	B	227	GLN
1	B	230	ASN
1	B	239	LYS
1	B	278	LEU
1	B	279	GLU
1	B	283	THR
1	B	290	GLN
1	B	294	SER
1	B	303	LYS
1	B	304	LEU
1	B	306	ILE
2	X	1	LYS
2	X	19	ASN
2	X	55	ILE

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Mol	Chain	Res	Type
2	X	73	LYS
2	X	75	LEU
2	X	103	ASN
2	X	118	THR
2	X	128	ARG
2	Y	1	LYS
2	Y	13	LYS
2	Y	19	ASN
2	Y	25	LEU
2	Y	41	HIS
2	Y	46	ASN
2	Y	50	SER
2	Y	55	ILE
2	Y	60	SER
2	Y	73	LYS
2	Y	75	LEU
2	Y	78	ILE
2	Y	85	SER
2	Y	88	ILE
2	Y	91	SER
2	Y	103	ASN
2	Y	125	ARG
2	Y	129	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	35	HIS
1	A	39	GLN
1	A	43	GLN
1	A	77	ASN
1	A	82	GLN
1	A	108	GLN
1	A	227	GLN
1	A	237	GLN
1	A	238	GLN
1	A	290	GLN
1	A	291	HIS
1	B	1	GLN
1	B	6	GLN
1	B	35	HIS

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Mol	Chain	Res	Type
1	B	43	GLN
1	B	77	ASN
1	B	108	GLN
1	B	237	GLN
1	B	290	GLN
1	B	291	HIS
2	X	19	ASN
2	X	46	ASN
2	X	57	GLN
2	X	59	ASN
2	X	65	ASN
2	X	77	ASN
2	X	93	ASN
2	X	103	ASN
2	X	121	HIS
2	Y	44	ASN
2	Y	59	ASN
2	Y	93	ASN
2	Y	103	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	224/253 (88%)	0.64	28 (12%) 8 7	15, 27, 70, 80	0
1	B	224/253 (88%)	0.60	26 (11%) 9 8	11, 24, 68, 79	0
2	X	129/129 (100%)	-0.14	2 (1%) 70 70	12, 20, 32, 51	1 (0%)
2	Y	129/129 (100%)	1.41	41 (31%) 1 1	15, 43, 73, 80	0
All	All	706/764 (92%)	0.63	97 (13%) 6 6	11, 27, 69, 80	1 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	ILE	8.6
1	A	215	LEU	6.9
1	A	228	ASP	6.6
1	A	7	SER	6.6
1	B	228	ASP	6.3
1	A	229	ILE	5.7
1	B	277	SER	5.5
1	B	215	LEU	5.4
2	Y	129	LEU	4.7
1	B	227	GLN	4.6
2	Y	83	LEU	4.5
1	B	212	TYR	4.5
1	B	230	ASN	4.4
1	A	216	GLY	4.3
1	B	117	GLY	4.3
1	B	116	SER	4.3
1	A	277	SER	4.3
1	A	230	ASN	4.1
1	B	226	SER	4.1
2	Y	47	THR	4.1
2	Y	53	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	216	GLY	3.9
1	A	279	GLU	3.9
2	Y	127	CYS	3.8
2	Y	126	GLY	3.8
1	B	278	LEU	3.7
1	A	226	SER	3.7
2	Y	48	ASP	3.6
2	Y	50	SER	3.5
1	B	261	ARG	3.5
1	B	281	ASP	3.4
2	Y	84	LEU	3.3
2	Y	40	THR	3.2
1	B	306	ILE	3.2
1	B	213	THR	3.2
2	Y	46	ASN	3.1
1	A	8	GLY	3.0
1	A	1	GLN	3.0
1	A	278	LEU	2.9
1	A	281	ASP	2.9
2	Y	36	SER	2.8
1	B	211	MET	2.8
1	B	279	GLU	2.8
1	A	225	ALA	2.8
1	A	306	ILE	2.8
1	B	210	SER	2.7
2	Y	51	THR	2.7
1	A	227	GLN	2.7
1	A	284	THR	2.7
2	Y	38	PHE	2.7
1	A	276	SER	2.7
2	Y	2	VAL	2.7
1	B	292	GLY	2.7
2	X	62	TRP	2.7
2	Y	9	ALA	2.6
2	Y	70	PRO	2.6
1	A	202	ILE	2.6
2	Y	4	GLY	2.6
1	A	239	LYS	2.6
1	B	276	SER	2.6
2	Y	39	ASN	2.5
2	Y	79	PRO	2.5
2	Y	90	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	Y	88	ILE	2.5
1	B	115	SER	2.5
2	Y	71	GLY	2.5
2	Y	64	CYS	2.4
1	B	280	SER	2.4
2	Y	44	ASN	2.4
2	Y	72	SER	2.4
2	Y	14	ARG	2.4
2	Y	68	ARG	2.4
2	Y	25	LEU	2.3
2	Y	49	GLY	2.3
2	Y	124	ILE	2.3
2	Y	6	CYS	2.3
1	A	211	MET	2.3
1	A	280	SER	2.3
1	A	261	ARG	2.3
2	Y	10	ALA	2.3
2	X	41	HIS	2.2
2	Y	3	TYR	2.2
1	A	116	SER	2.2
1	B	208	PRO	2.2
1	B	8	GLY	2.2
2	Y	125	ARG	2.2
1	A	208	PRO	2.1
2	Y	77	ASN	2.1
2	Y	45	ARG	2.1
2	Y	16	GLY	2.1
1	A	241	GLY	2.1
1	B	258	VAL	2.1
2	Y	128	ARG	2.0
1	A	209	SER	2.0
2	Y	42	ALA	2.0
2	Y	59	ASN	2.0
1	A	213	THR	2.0

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

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.