



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:58 AM UTC

PDB ID : 1BZ7 / pdb_00001bz7
Title : FAB FRAGMENT FROM MURINE ASCITES
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Deposited on : 1998-11-06
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

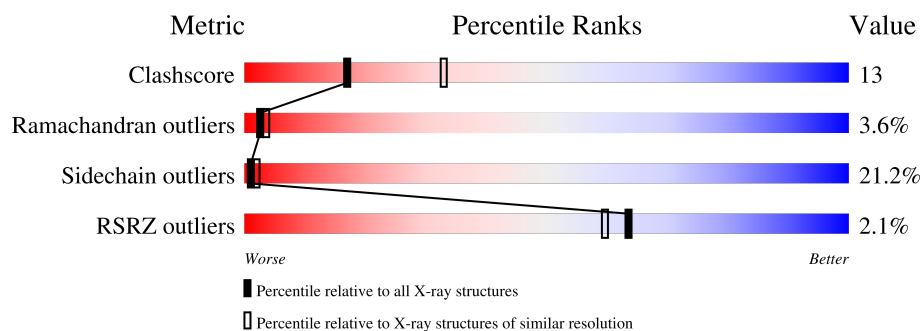
1 Overall quality at a glance

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))
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	206	
2	B	217	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3232 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN (ANTIBODY R24 (LIGHT CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1598	1004	264	325	5			

- Molecule 2 is a protein called PROTEIN (ANTIBODY R24 (HEAVY CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1621	1023	273	319	6			

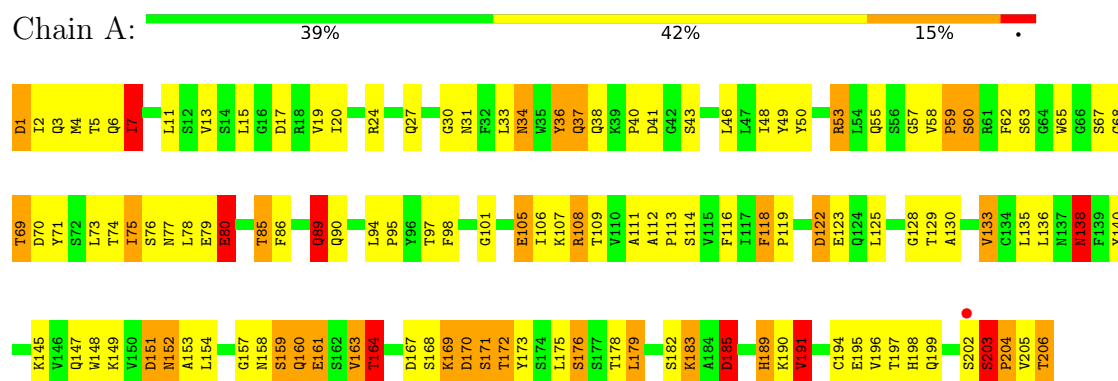
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	6	Total	O	0	0
			6	6		

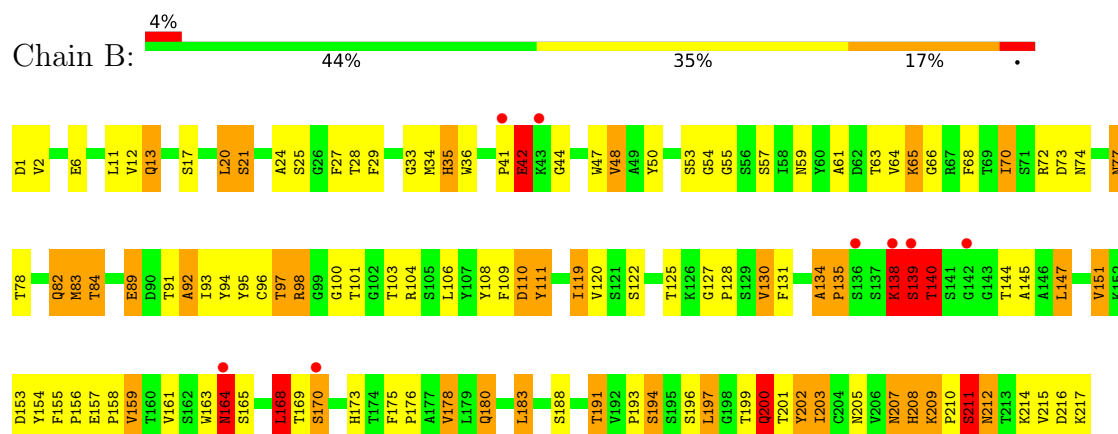
3 Residue-property plots [i](#)

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: PROTEIN (ANTIBODY R24 (LIGHT CHAIN))



• Molecule 2: PROTEIN (ANTIBODY R24 (HEAVY CHAIN))



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.80Å 56.00Å 80.00Å 90.00° 119.20° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50 6.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.0 (6.00-2.50) 81.5 (6.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.162 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3232	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% 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	1.28	6/1630 (0.4%)	2.27	92/2210 (4.2%)
2	B	1.29	10/1661 (0.6%)	2.35	93/2259 (4.1%)
All	All	1.29	16/3291 (0.5%)	2.31	185/4469 (4.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
All	All	0	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	151	VAL	CA-CB	8.85	1.64	1.53
1	A	198	HIS	CD2-NE2	-7.65	1.29	1.37
2	B	208	HIS	CD2-NE2	-7.39	1.29	1.37
1	A	189	HIS	CD2-NE2	-6.72	1.30	1.37
2	B	164	ASN	CA-CB	6.28	1.63	1.53
2	B	173	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	59	PRO	CA-CB	-6.08	1.45	1.53
2	B	35	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	75	ILE	CA-CB	-5.73	1.47	1.53
1	A	195	GLU	CA-CB	-5.37	1.45	1.53
2	B	178	VAL	CA-CB	5.33	1.60	1.54
1	A	38	GLN	CA-CB	-5.22	1.45	1.53
2	B	47	TRP	CG-CD2	-5.21	1.34	1.43
2	B	140	THR	CA-CB	5.12	1.62	1.53
2	B	173	HIS	CG-ND1	-5.12	1.32	1.38
2	B	70	ILE	CA-CB	5.09	1.61	1.54

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	164	ASN	CA-CB-CG	14.12	126.72	112.60
2	B	73	ASP	CA-CB-CG	11.73	124.33	112.60
1	A	2	ILE	N-CA-C	-11.71	91.77	108.17
1	A	2	ILE	N-CA-CB	-11.53	95.57	111.25
1	A	170	ASP	CA-CB-CG	11.49	124.09	112.60
1	A	189	HIS	CB-CG-CD2	-10.71	117.28	131.20
2	B	100	GLY	N-CA-C	9.76	125.27	112.77
2	B	153	ASP	N-CA-C	9.69	122.25	110.91
1	A	189	HIS	CB-CG-ND1	9.53	137.00	122.70
2	B	42	GLU	N-CA-C	-9.51	90.55	110.80
2	B	208	HIS	CA-CB-CG	9.21	123.01	113.80
2	B	211	SER	N-CA-C	9.14	130.27	110.80
1	A	70	ASP	N-CA-C	9.13	123.81	108.20
2	B	211	SER	O-C-N	9.08	134.67	122.59
1	A	171	SER	N-CA-C	8.96	123.71	112.24
2	B	134	ALA	N-CA-C	8.79	123.59	110.32
1	A	147	GLN	OE1-CD-NE2	-8.73	113.87	122.60
2	B	64	VAL	N-CA-C	-8.57	104.54	112.43
2	B	98	ARG	CB-CG-CD	-8.50	91.75	111.30
2	B	208	HIS	CB-CG-CD2	-8.47	120.19	131.20
2	B	110	ASP	CA-CB-CG	8.43	121.03	112.60
1	A	80	GLU	CB-CG-CD	8.39	126.87	112.60
2	B	164	ASN	OD1-CG-ND2	-8.36	114.24	122.60
2	B	170	SER	N-CA-C	-8.29	99.88	111.81
2	B	165	SER	N-CA-C	-8.21	97.33	109.15
1	A	179	LEU	N-CA-C	-8.17	95.09	108.41
1	A	2	ILE	CB-CA-C	8.07	122.85	110.83
1	A	122	ASP	CA-CB-CG	8.05	120.65	112.60
2	B	29	PHE	CA-CB-CG	7.96	121.77	113.80
2	B	217	LYS	N-CA-CB	7.85	123.85	110.50
2	B	138	LYS	O-C-N	7.79	132.31	122.57
2	B	1	ASP	CA-CB-CG	7.73	120.33	112.60
2	B	35	HIS	CB-CG-CD2	-7.55	121.38	131.20
1	A	17	ASP	CA-CB-CG	7.54	120.14	112.60
1	A	58	VAL	N-CA-C	-7.53	99.17	108.05
1	A	37	GLN	OE1-CD-NE2	-7.52	115.08	122.60
2	B	13	GLN	OE1-CD-NE2	-7.50	115.10	122.60
1	A	205	VAL	CA-C-O	-7.49	113.92	121.49
2	B	83	MET	CG-SD-CE	-7.42	84.56	100.90
1	A	1	ASP	CA-C-O	7.42	133.41	120.80
2	B	44	GLY	O-C-N	7.25	129.90	122.79
1	A	172	THR	N-CA-CB	-7.24	99.91	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	LEU	N-CA-C	7.17	117.85	109.60
2	B	211	SER	CA-C-N	7.13	135.15	121.54
2	B	211	SER	C-N-CA	7.13	135.15	121.54
2	B	97	THR	CA-CB-OG1	-7.10	98.95	109.60
2	B	209	LYS	N-CA-C	7.05	125.40	109.81
1	A	7	ILE	CB-CG1-CD1	6.97	128.43	113.80
1	A	89	GLN	CG-CD-NE2	-6.95	105.98	116.40
1	A	164	THR	N-CA-CB	-6.93	100.44	110.36
2	B	208	HIS	CB-CG-ND1	6.93	133.09	122.70
1	A	69	THR	N-CA-CB	6.91	120.70	110.33
2	B	101	THR	CA-CB-OG1	-6.88	99.29	109.60
1	A	185	ASP	CA-CB-CG	-6.84	105.76	112.60
1	A	118	PHE	CA-CB-CG	6.78	120.58	113.80
1	A	198	HIS	CB-CG-CD2	-6.75	122.42	131.20
2	B	100	GLY	CA-C-O	-6.74	113.52	120.66
2	B	68	PHE	CA-CB-CG	6.67	120.47	113.80
1	A	13	VAL	N-CA-CB	-6.66	103.20	112.52
1	A	206	THR	N-CA-CB	-6.65	100.19	111.50
1	A	123	GLU	CA-CB-CG	6.65	127.39	114.10
2	B	202	TYR	CA-C-O	-6.63	113.20	120.43
1	A	37	GLN	CG-CD-NE2	6.61	126.32	116.40
2	B	201	THR	N-CA-CB	-6.58	99.66	110.52
2	B	164	ASN	CB-CG-ND2	6.58	126.27	116.40
2	B	159	VAL	CB-CA-C	-6.55	101.41	111.31
2	B	59	ASN	OD1-CG-ND2	-6.55	116.05	122.60
2	B	95	TYR	CA-C-O	-6.55	113.77	120.71
1	A	34	ASN	OD1-CG-ND2	-6.55	116.05	122.60
2	B	135	PRO	N-CA-C	6.54	125.94	112.47
1	A	122	ASP	CA-C-N	6.50	128.90	120.44
1	A	122	ASP	C-N-CA	6.50	128.90	120.44
1	A	152	ASN	CA-CB-CG	-6.48	106.12	112.60
1	A	3	GLN	CA-C-O	-6.47	113.37	120.81
2	B	180	GLN	N-CA-C	-6.41	99.92	109.86
1	A	73	LEU	N-CA-C	-6.39	98.99	109.40
1	A	41	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	198	HIS	CB-CG-ND1	6.23	132.04	122.70
1	A	90	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	A	136	LEU	N-CA-C	-6.22	98.38	108.52
1	A	157	GLY	N-CA-C	6.22	124.80	114.48
2	B	33	GLY	N-CA-C	-6.21	104.12	112.14
1	A	205	VAL	N-CA-CB	-6.20	102.15	112.06
2	B	216	ASP	N-CA-C	6.18	116.73	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ASN	OD1-CG-ND2	-6.17	116.42	122.60
1	A	6	GLN	N-CA-C	-6.17	95.29	107.69
1	A	167	ASP	CA-CB-CG	6.15	118.75	112.60
2	B	97	THR	N-CA-CB	-6.14	100.11	111.53
1	A	138	ASN	N-CA-C	6.10	123.78	110.80
2	B	168	LEU	CA-C-O	6.08	129.21	120.51
2	B	130	VAL	O-C-N	-6.07	116.49	122.93
2	B	202	TYR	O-C-N	-6.06	116.42	123.27
1	A	163	VAL	N-CA-C	-6.06	99.43	108.46
2	B	97	THR	CA-CB-CG2	6.02	120.74	110.50
2	B	13	GLN	CB-CG-CD	6.02	122.83	112.60
1	A	98	PHE	CA-CB-CG	6.02	119.82	113.80
1	A	79	GLU	CA-C-N	5.98	128.58	120.38
1	A	79	GLU	C-N-CA	5.98	128.58	120.38
2	B	131	PHE	CA-C-N	5.98	125.94	119.78
2	B	131	PHE	C-N-CA	5.98	125.94	119.78
1	A	169	LYS	N-CA-C	-5.94	100.87	110.32
2	B	217	LYS	CB-CA-C	-5.93	98.83	110.10
2	B	93	ILE	N-CA-CB	5.85	118.06	111.21
2	B	92	ALA	CA-C-O	-5.84	114.88	121.25
1	A	4	MET	O-C-N	-5.81	116.70	123.27
2	B	163	TRP	CA-C-O	5.81	128.82	120.51
2	B	89	GLU	N-CA-C	5.78	120.02	113.15
2	B	96	CYS	CA-C-O	5.77	127.20	120.80
1	A	76	SER	CA-C-O	-5.76	114.96	120.90
2	B	101	THR	CA-CB-CG2	5.73	120.25	110.50
1	A	170	ASP	N-CA-C	5.72	122.98	110.80
2	B	35	HIS	CB-CG-ND1	5.71	131.26	122.70
1	A	161	GLU	N-CA-C	5.69	118.76	108.69
2	B	207	ASN	O-C-N	-5.68	117.00	123.48
1	A	203	SER	N-CA-C	-5.67	97.27	109.81
1	A	164	THR	CA-CB-OG1	-5.66	101.10	109.60
1	A	160	GLN	N-CA-C	-5.66	100.56	109.50
1	A	107	LYS	O-C-N	5.66	129.72	123.16
1	A	20	ILE	CB-CG1-CD1	5.61	125.58	113.80
1	A	140	TYR	O-C-N	-5.61	117.45	121.83
2	B	147	LEU	O-C-N	-5.56	116.44	123.17
2	B	191	THR	N-CA-C	-5.55	99.37	108.41
2	B	139	SER	N-CA-C	5.54	122.59	110.80
2	B	13	GLN	CG-CD-NE2	5.54	124.70	116.40
1	A	7	ILE	CA-CB-CG1	5.53	119.80	110.40
2	B	84	THR	N-CA-CB	-5.51	102.09	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47	TRP	CA-C-N	-5.51	117.51	123.08
2	B	47	TRP	C-N-CA	-5.51	117.51	123.08
2	B	168	LEU	N-CA-C	5.51	122.54	110.80
1	A	170	ASP	O-C-N	-5.50	115.27	122.59
2	B	34	MET	CG-SD-CE	-5.48	88.85	100.90
2	B	175	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	1	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	85	THR	CB-CA-C	5.44	120.12	109.35
2	B	63	THR	N-CA-CB	-5.42	101.98	110.44
1	A	148	TRP	CE2-CD2-CG	-5.41	100.71	107.20
2	B	180	GLN	O-C-N	-5.40	114.92	121.83
1	A	191	VAL	CA-CB-CG2	-5.40	101.22	110.40
1	A	67	SER	CB-CA-C	-5.39	103.58	111.77
2	B	82	GLN	OE1-CD-NE2	-5.37	117.23	122.60
2	B	163	TRP	CA-CB-CG	5.36	123.79	113.60
1	A	138	ASN	OD1-CG-ND2	-5.36	117.24	122.60
2	B	106	LEU	N-CA-C	-5.36	100.50	109.24
1	A	55	GLN	N-CA-CB	-5.36	102.46	110.17
2	B	1	ASP	CA-C-O	-5.33	111.74	120.80
1	A	7	ILE	CA-CB-CG2	-5.32	101.45	110.50
1	A	73	LEU	O-C-N	5.32	130.15	123.23
2	B	134	ALA	CA-C-N	5.30	126.47	119.84
2	B	134	ALA	C-N-CA	5.30	126.47	119.84
1	A	27	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	A	89	GLN	CG-CD-OE1	5.30	131.40	120.80
2	B	77	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	130	ALA	CA-C-O	-5.28	114.86	120.40
1	A	167	ASP	CA-C-N	5.28	127.30	120.44
1	A	167	ASP	C-N-CA	5.28	127.30	120.44
1	A	122	ASP	O-C-N	5.27	129.60	122.59
1	A	119	PRO	CB-CA-C	5.26	117.34	110.92
1	A	106	ILE	N-CA-CB	-5.26	104.79	110.53
1	A	160	GLN	OE1-CD-NE2	-5.25	117.35	122.60
2	B	78	THR	OG1-CB-CG2	-5.25	98.81	109.30
2	B	200	GLN	CA-CB-CG	5.24	124.58	114.10
2	B	163	TRP	CD1-CG-CD2	5.23	114.67	106.30
2	B	211	SER	CA-CB-OG	-5.23	100.63	111.10
2	B	48	VAL	N-CA-CB	-5.21	105.68	111.41
1	A	27	GLN	CG-CD-NE2	5.21	124.22	116.40
1	A	70	ASP	CA-CB-CG	-5.19	107.41	112.60
1	A	202	SER	N-CA-C	-5.19	99.53	108.56
1	A	111	ALA	N-CA-C	-5.18	101.24	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	GLN	CA-CB-CG	5.15	124.41	114.10
2	B	194	SER	CA-C-N	5.15	127.90	120.38
2	B	194	SER	C-N-CA	5.15	127.90	120.38
2	B	173	HIS	N-CA-C	-5.14	98.91	107.80
2	B	111	TYR	CA-C-O	-5.12	114.46	120.60
1	A	183	LYS	N-CA-C	-5.08	105.66	111.14
1	A	151	ASP	N-CA-C	-5.07	104.43	111.52
2	B	163	TRP	CG-CD1-NE1	-5.07	103.61	110.20
1	A	105	GLU	N-CA-C	-5.05	101.53	109.50
2	B	217	LYS	CB-CG-CD	-5.04	99.70	111.30
2	B	128	PRO	N-CA-C	5.04	118.96	111.41
2	B	20	LEU	N-CA-C	-5.03	102.63	110.42
2	B	61	ALA	N-CA-C	-5.03	103.04	110.48
2	B	82	GLN	CB-CG-CD	5.02	121.13	112.60
1	A	57	GLY	CA-C-N	-5.01	118.43	123.04
1	A	57	GLY	C-N-CA	-5.01	118.43	123.04
1	A	160	GLN	CG-CD-NE2	5.01	123.91	116.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	SER	Peptide
1	A	36	TYR	Sidechain
2	B	111	TYR	Sidechain
2	B	210	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	1598	0	1559	38	0
2	B	1621	0	1580	46	0
3	A	7	0	0	0	0
3	B	6	0	0	0	0
All	All	3232	0	3139	81	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 13.

All (81) 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)
2:B:20:LEU:HD13	2:B:83:MET:HE1	1.35	1.08
2:B:11:LEU:HD11	2:B:155:PHE:HE1	1.52	0.73
2:B:196:SER:HB3	2:B:200:GLN:HE22	1.52	0.72
1:A:159:SER:HA	1:A:178:THR:O	1.94	0.68
2:B:164:ASN:HD21	2:B:170:SER:HA	1.60	0.67
1:A:163:VAL:HG12	1:A:164:THR:O	1.95	0.66
2:B:20:LEU:CD1	2:B:83:MET:HE1	2.21	0.64
2:B:65:LYS:HE3	2:B:66:GLY:N	2.12	0.64
2:B:138:LYS:HA	2:B:194:SER:HB3	1.80	0.64
2:B:12:VAL:O	2:B:120:VAL:HA	1.99	0.62
1:A:145:LYS:HB3	1:A:197:THR:HB	1.81	0.62
1:A:86:PHE:O	1:A:101:GLY:HA2	2.00	0.61
1:A:118:PHE:HB2	1:A:133:VAL:HG22	1.82	0.60
2:B:2:VAL:HG13	2:B:27:PHE:CD1	2.36	0.60
2:B:11:LEU:HD11	2:B:155:PHE:CE1	2.37	0.60
2:B:72:ARG:NE	2:B:74:ASN:HD21	2.01	0.58
2:B:161:VAL:HG11	2:B:188:SER:CB	2.33	0.58
2:B:97:THR:OG1	2:B:109:PHE:HB3	2.03	0.58
1:A:116:PHE:CD1	2:B:140:THR:HB	2.39	0.57
2:B:91:THR:HG23	2:B:119:ILE:HA	1.87	0.56
2:B:98:ARG:HD3	2:B:110:ASP:OD1	2.06	0.55
1:A:31:ASN:HB3	1:A:50:TYR:CE1	2.43	0.53
1:A:116:PHE:HD1	2:B:140:THR:HB	1.73	0.52
1:A:185:ASP:O	1:A:189:HIS:CD2	2.64	0.51
1:A:53:ARG:NE	1:A:53:ARG:HA	2.26	0.51
2:B:72:ARG:HE	2:B:74:ASN:ND2	2.09	0.51
1:A:1:ASP:HB2	1:A:95:PRO:HD2	1.93	0.51
2:B:41:PRO:O	2:B:42:GLU:HB2	2.11	0.51
1:A:19:VAL:HG21	1:A:78:LEU:HD13	1.93	0.51
1:A:149:LYS:HA	1:A:153:ALA:O	2.12	0.49
1:A:34:ASN:ND2	2:B:108:TYR:HB3	2.28	0.49
1:A:151:ASP:HA	1:A:191:VAL:HG12	1.93	0.49
2:B:145:ALA:CB	2:B:197:LEU:HD21	2.43	0.49
1:A:128:GLY:HA2	1:A:183:LYS:HB2	1.94	0.49
2:B:196:SER:HB3	2:B:202:TYR:OH	2.13	0.49
1:A:33:LEU:HD22	1:A:71:TYR:CD2	2.48	0.49
1:A:182:SER:OG	1:A:185:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:HIS:CE1	2:B:50:TYR:CD1	3.01	0.48
2:B:92:ALA:HB3	2:B:94:TYR:CE1	2.49	0.48
2:B:205:ASN:HB3	2:B:215:VAL:HG12	1.95	0.48
1:A:161:GLU:HA	1:A:176:SER:O	2.14	0.48
2:B:139:SER:HB2	2:B:145:ALA:HA	1.95	0.47
1:A:194:CYS:O	1:A:206:THR:HA	2.14	0.47
1:A:108:ARG:HG2	1:A:171:SER:CB	2.44	0.47
1:A:49:TYR:O	1:A:53:ARG:HB2	2.14	0.46
2:B:161:VAL:HG11	2:B:188:SER:HB2	1.96	0.46
1:A:59:PRO:HG2	1:A:62:PHE:CE1	2.50	0.46
1:A:196:VAL:O	1:A:204:PRO:HA	2.15	0.46
1:A:7:ILE:HD12	1:A:7:ILE:H	1.80	0.46
2:B:65:LYS:HA	2:B:65:LYS:HD2	1.56	0.45
2:B:145:ALA:HB1	2:B:197:LEU:HD21	1.98	0.45
1:A:33:LEU:HD22	1:A:71:TYR:CG	2.52	0.45
1:A:80:GLU:H	1:A:80:GLU:CD	2.24	0.45
1:A:138:ASN:HA	1:A:173:TYR:O	2.16	0.45
1:A:59:PRO:HG2	1:A:62:PHE:CD1	2.52	0.45
1:A:37:GLN:HG3	1:A:86:PHE:CE1	2.51	0.45
2:B:130:VAL:HG21	2:B:214:LYS:HG2	1.99	0.44
2:B:211:SER:OG	2:B:212:ASN:N	2.50	0.44
1:A:19:VAL:O	1:A:74:THR:HA	2.18	0.44
2:B:24:ALA:HB1	2:B:27:PHE:CZ	2.53	0.44
2:B:36:TRP:O	2:B:48:VAL:HB	2.17	0.44
1:A:36:TYR:HE2	1:A:89:GLN:HG2	1.83	0.43
1:A:48:ILE:HA	1:A:53:ARG:O	2.19	0.43
2:B:209:LYS:HB3	2:B:209:LYS:HE2	1.73	0.43
1:A:75:ILE:HG21	1:A:78:LEU:HD12	2.00	0.43
2:B:203:ILE:HG22	2:B:205:ASN:ND2	2.33	0.43
1:A:108:ARG:HG2	1:A:171:SER:HB2	2.01	0.43
2:B:154:TYR:O	2:B:183:LEU:HB3	2.19	0.43
1:A:36:TYR:O	1:A:86:PHE:HA	2.19	0.42
2:B:72:ARG:NE	2:B:74:ASN:ND2	2.67	0.42
2:B:17:SER:HB3	2:B:82:GLN:HE22	1.85	0.42
2:B:127:GLY:HA2	2:B:208:HIS:CD2	2.55	0.42
2:B:144:THR:HA	2:B:193:PRO:HA	2.00	0.42
1:A:163:VAL:CG2	1:A:175:LEU:HD12	2.49	0.42
1:A:112:ALA:HA	1:A:113:PRO:HD3	1.81	0.41
2:B:139:SER:OG	2:B:197:LEU:HD11	2.21	0.41
2:B:70:ILE:HD13	2:B:70:ILE:HG21	1.87	0.41
2:B:125:THR:HA	2:B:155:PHE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:ALA:HA	2:B:135:PRO:HD3	1.90	0.41
2:B:196:SER:O	2:B:199:THR:HB	2.22	0.40
2:B:6:GLU:HA	2:B:21:SER:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/206 (99%)	187 (92%)	10 (5%)	7 (3%)	3	4
2	B	215/217 (99%)	186 (86%)	21 (10%)	8 (4%)	2	3
All	All	419/423 (99%)	373 (89%)	31 (7%)	15 (4%)	2	3

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
2	B	42	GLU
2	B	139	SER
2	B	140	THR
2	B	168	LEU
2	B	211	SER
2	B	212	ASN
1	A	30	GLY
1	A	60	SER
1	A	68	GLY
1	A	138	ASN
2	B	55	GLY
1	A	199	GLN
2	B	54	GLY
1	A	203	SER

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	183/183 (100%)	142 (78%)	41 (22%)	1	2
2	B	180/180 (100%)	144 (80%)	36 (20%)	1	2
All	All	363/363 (100%)	286 (79%)	77 (21%)	1	2

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	7	ILE
1	A	11	LEU
1	A	15	LEU
1	A	24	ARG
1	A	40	PRO
1	A	43	SER
1	A	46	LEU
1	A	53	ARG
1	A	60	SER
1	A	63	SER
1	A	65	TRP
1	A	69	THR
1	A	80	GLU
1	A	85	THR
1	A	89	GLN
1	A	97	THR
1	A	105	GLU
1	A	108	ARG
1	A	109	THR
1	A	114	SER
1	A	125	LEU
1	A	129	THR
1	A	133	VAL
1	A	135	LEU
1	A	152	ASN
1	A	154	LEU

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Mol	Chain	Res	Type
1	A	158	ASN
1	A	159	SER
1	A	160	GLN
1	A	164	THR
1	A	168	SER
1	A	169	LYS
1	A	170	ASP
1	A	172	THR
1	A	176	SER
1	A	179	LEU
1	A	185	ASP
1	A	190	LYS
1	A	191	VAL
1	A	204	PRO
2	B	13	GLN
2	B	21	SER
2	B	25	SER
2	B	28	THR
2	B	42	GLU
2	B	53	SER
2	B	57	SER
2	B	65	LYS
2	B	77	ASN
2	B	84	THR
2	B	89	GLU
2	B	103	THR
2	B	104	ARG
2	B	119	ILE
2	B	122	SER
2	B	138	LYS
2	B	140	THR
2	B	147	LEU
2	B	151	VAL
2	B	156	PRO
2	B	157	GLU
2	B	158	PRO
2	B	159	VAL
2	B	164	ASN
2	B	168	LEU
2	B	169	THR
2	B	176	PRO
2	B	178	VAL

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Mol	Chain	Res	Type
2	B	180	GLN
2	B	183	LEU
2	B	191	THR
2	B	197	LEU
2	B	200	GLN
2	B	203	ILE
2	B	207	ASN
2	B	211	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	89	GLN
1	A	152	ASN
1	A	158	ASN
1	A	189	HIS
2	B	31	ASN
2	B	74	ASN
2	B	82	GLN
2	B	164	ASN
2	B	173	HIS
2	B	180	GLN
2	B	205	ASN
2	B	208	HIS
2	B	212	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	206/206 (100%)	-0.61	1 (0%) 87 85	5, 25, 52, 73	0
2	B	217/217 (100%)	-0.42	8 (3%) 45 40	3, 23, 80, 111	0
All	All	423/423 (100%)	-0.51	9 (2%) 63 59	3, 24, 64, 111	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	142	GLY	4.1
2	B	136	SER	3.5
2	B	170	SER	2.6
1	A	202	SER	2.5
2	B	138	LYS	2.3
2	B	43	LYS	2.2
2	B	41	PRO	2.2
2	B	139	SER	2.2
2	B	164	ASN	2.1

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.