



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:53 PM UTC

PDB ID : 3BTN / pdb_00003btn
Title : Crystal structure of antizyme inhibitor, an ornithine decarboxylase homologous protein
Authors : Dym, O.; Unger, T.; Albeck, S.; Kahana, C.; Israel Structural Proteomics Center (ISPC)
Deposited on : 2007-12-30
Resolution : 2.05 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

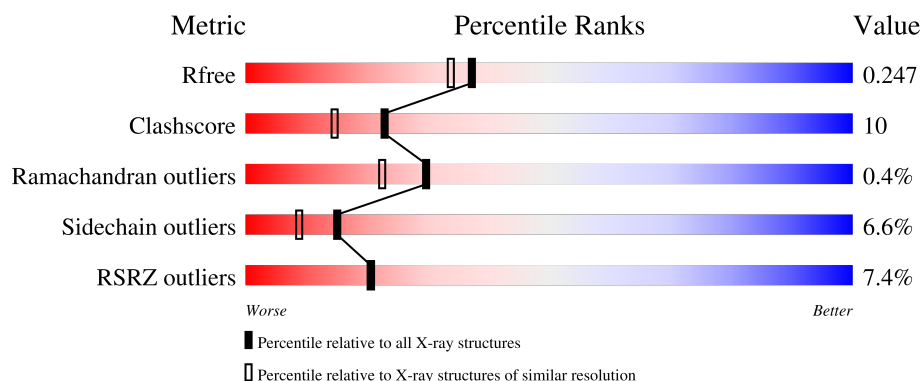
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	448	
1	B	448	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6283 atoms, of which 0 are hydrogens and 0 are deuteriums.

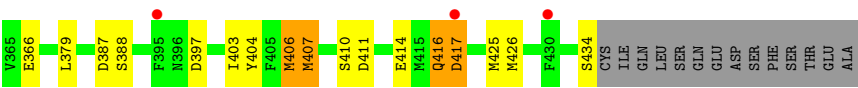
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Antizyme inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	1	0
			3044	1964	486	569	25			
1	B	390	Total	C	N	O	S	0	3	0
			3047	1965	484	574	24			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	104	Total	O	0	0
			104	104		
2	B	88	Total	O	0	0
			88	88		



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	92.77Å 98.39Å 117.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.05 50.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.05) 99.9 (50.00-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.241 (Not available) , 0.247	Depositor DCC
R_{free} test set	3477 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6283	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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	1.96	53/3115 (1.7%)	1.59	36/4217 (0.9%)
1	B	1.87	46/3125 (1.5%)	1.48	30/4230 (0.7%)
All	All	1.92	99/6240 (1.6%)	1.54	66/8447 (0.8%)

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	3

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	ILE	CA-CB	9.62	1.61	1.54
1	A	425	MET	SD-CE	-8.97	1.57	1.79
1	A	99	GLN	N-CA	8.04	1.56	1.46
1	A	209	VAL	CA-CB	7.96	1.63	1.54
1	B	280	ALA	CA-C	7.78	1.63	1.52
1	A	220	ASP	N-CA	7.49	1.54	1.46
1	B	387	ASP	CB-CG	7.38	1.70	1.52
1	B	189	VAL	CA-CB	7.36	1.63	1.54
1	B	198	VAL	CA-CB	7.23	1.63	1.54
1	B	122	TYR	CA-CB	7.19	1.64	1.53
1	B	41	PHE	C-O	7.16	1.32	1.23
1	A	60	ALA	CA-CB	7.13	1.65	1.53
1	B	425	MET	CA-C	7.05	1.62	1.52
1	B	98	VAL	CA-CB	6.95	1.63	1.54
1	B	209	VAL	C-O	-6.93	1.16	1.24
1	A	103	VAL	CA-CB	6.83	1.61	1.54
1	A	48	ILE	CA-CB	6.79	1.63	1.54
1	B	88	ALA	CA-C	6.69	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	SER	CA-C	6.68	1.61	1.52
1	B	194	VAL	C-O	-6.65	1.17	1.23
1	A	211	ALA	N-CA	6.62	1.54	1.46
1	A	192	ILE	CA-CB	6.61	1.61	1.54
1	B	73	THR	CA-C	6.58	1.60	1.53
1	A	55	TRP	CA-CB	6.54	1.63	1.53
1	B	215	ALA	N-CA	6.54	1.54	1.46
1	A	85	THR	N-CA	6.54	1.54	1.45
1	B	141	LYS	C-O	-6.54	1.16	1.24
1	B	178	ARG	CG-CD	6.48	1.71	1.52
1	A	325	ALA	CA-CB	6.48	1.63	1.53
1	B	407	MET	CA-C	6.42	1.60	1.52
1	B	387	ASP	CA-CB	6.38	1.62	1.53
1	A	386	ALA	CA-CB	6.37	1.64	1.53
1	B	277	VAL	N-CA	6.34	1.52	1.46
1	A	400	ARG	CZ-NH2	6.24	1.41	1.33
1	B	211	ALA	CA-CB	6.24	1.63	1.53
1	A	57	THR	N-CA	6.22	1.53	1.46
1	A	171	GLY	N-CA	-6.20	1.39	1.45
1	A	424	ALA	CA-CB	6.19	1.63	1.53
1	B	403	ILE	CB-CG2	6.17	1.73	1.52
1	A	173	THR	CA-CB	6.16	1.63	1.53
1	B	218	VAL	CA-CB	6.14	1.62	1.54
1	B	268	ILE	CA-C	6.10	1.60	1.52
1	B	216	ARG	N-CA	6.06	1.53	1.46
1	A	200	SER	N-CA	6.01	1.53	1.46
1	A	72	SER	N-CA	5.98	1.53	1.46
1	A	157	THR	CA-C	5.97	1.59	1.52
1	A	394	ALA	N-CA	5.94	1.53	1.46
1	A	424	ALA	C-O	-5.93	1.16	1.24
1	B	245	LEU	CA-C	5.91	1.60	1.52
1	B	49	VAL	CA-C	5.83	1.60	1.52
1	B	242	GLU	N-CA	5.83	1.53	1.46
1	A	25	ILE	CA-CB	-5.78	1.47	1.54
1	A	59	VAL	N-CA	5.77	1.53	1.46
1	A	59	VAL	CA-CB	5.75	1.62	1.54
1	A	413	TYR	N-CA	5.71	1.53	1.46
1	B	90	SER	N-CA	-5.70	1.39	1.46
1	A	237	GLY	N-CA	5.69	1.53	1.45
1	A	253	SER	N-CA	-5.69	1.41	1.46
1	B	154	HIS	C-O	-5.63	1.17	1.24
1	A	339	HIS	N-CA	-5.59	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	THR	CA-C	5.57	1.59	1.53
1	A	117	VAL	CA-CB	5.55	1.61	1.54
1	A	120	ILE	CA-CB	5.51	1.61	1.54
1	A	50	LYS	C-O	5.48	1.30	1.24
1	B	87	PHE	C-O	-5.46	1.17	1.23
1	B	35	THR	CA-CB	5.44	1.62	1.53
1	A	80	LEU	N-CA	5.44	1.53	1.46
1	B	103	VAL	N-CA	5.44	1.52	1.46
1	A	74	PRO	C-O	-5.40	1.17	1.24
1	B	142	ILE	CA-CB	5.40	1.60	1.54
1	A	92	LYS	CA-CB	5.36	1.61	1.53
1	A	404	TYR	N-CA	5.36	1.52	1.46
1	A	282	THR	N-CA	5.35	1.52	1.46
1	A	277	VAL	CA-CB	5.33	1.61	1.54
1	A	385	GLY	N-CA	5.31	1.52	1.45
1	B	124	ALA	CA-C	5.30	1.59	1.52
1	A	266	ILE	CA-CB	-5.29	1.47	1.54
1	B	143	ALA	CA-CB	5.28	1.61	1.53
1	A	158	GLU	N-CA	5.28	1.53	1.46
1	B	245	LEU	N-CA	-5.24	1.40	1.46
1	B	19	THR	CA-C	5.24	1.59	1.52
1	A	260	PHE	CA-C	5.22	1.59	1.52
1	A	428	ASN	C-O	5.22	1.30	1.24
1	B	335	ILE	N-CA	5.21	1.50	1.46
1	A	150	LYS	CA-C	-5.20	1.46	1.52
1	A	38	ASN	CA-C	5.19	1.59	1.52
1	B	183	CYS	N-CA	5.15	1.52	1.46
1	B	287	ILE	C-O	5.13	1.29	1.24
1	A	95	MET	CG-SD	5.12	1.93	1.80
1	B	82	ALA	N-CA	5.11	1.52	1.46
1	A	66	TYR	CA-CB	5.10	1.61	1.53
1	A	320	VAL	CB-CG2	-5.08	1.35	1.52
1	B	56	GLN	CA-C	5.08	1.59	1.52
1	B	272	PRO	CA-C	5.07	1.59	1.52
1	B	209	VAL	CB-CG1	5.06	1.69	1.52
1	A	396	ASN	CG-ND2	5.06	1.43	1.33
1	B	426	MET	C-O	-5.06	1.17	1.24
1	B	271	GLU	N-CA	5.04	1.51	1.46
1	A	13	GLY	N-CA	5.01	1.52	1.45

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	GLU	N-CA-C	-22.83	85.42	113.50
1	A	34	LEU	N-CA-C	-12.60	83.96	110.80
1	A	407	MET	CA-CB-CG	8.23	130.57	114.10
1	B	258	ILE	N-CA-C	7.59	117.66	110.53
1	B	85	THR	OG1-CB-CG2	7.58	124.46	109.30
1	A	109	ILE	CB-CG1-CD1	-7.56	97.92	113.80
1	A	258	ILE	N-CA-C	6.87	118.20	111.67
1	B	35	THR	N-CA-C	-6.82	96.28	110.80
1	A	111	THR	CB-CA-C	-6.60	100.33	111.02
1	B	357	SER	N-CA-C	6.58	120.90	113.01
1	A	36	GLY	N-CA-C	6.37	120.60	112.83
1	A	123	ALA	N-CA-C	6.29	118.65	111.11
1	B	171	GLY	N-CA-C	-6.24	106.02	111.95
1	B	271	GLU	CA-C-N	-6.23	113.56	119.85
1	B	271	GLU	C-N-CA	-6.23	113.56	119.85
1	B	131	MET	CA-CB-CG	6.14	126.38	114.10
1	A	370	LEU	N-CA-C	-6.06	99.70	109.58
1	B	151	VAL	N-CA-C	6.04	117.72	108.71
1	B	35	THR	CB-CA-C	6.03	122.43	110.42
1	B	60	ALA	N-CA-C	5.98	119.40	111.75
1	B	157	THR	OG1-CB-CG2	5.91	121.11	109.30
1	B	55	TRP	N-CA-C	-5.89	104.77	111.07
1	B	61	GLN	CB-CG-CD	5.88	122.60	112.60
1	B	36	GLY	N-CA-C	5.84	127.03	113.18
1	A	209	VAL	N-CA-C	5.83	116.02	110.42
1	A	257	ASP	CA-C-N	5.83	129.57	122.63
1	A	257	ASP	C-N-CA	5.83	129.57	122.63
1	B	222	ALA	CA-C-N	5.82	126.54	120.03
1	B	222	ALA	C-N-CA	5.82	126.54	120.03
1	A	146	HIS	CA-C-N	-5.74	113.90	119.87
1	A	146	HIS	C-N-CA	-5.74	113.90	119.87
1	A	99	GLN	CA-CB-CG	5.67	125.43	114.10
1	A	11	SER	CB-CA-C	5.66	119.09	109.75
1	B	19	THR	N-CA-C	5.63	118.71	109.76
1	B	388	SER	N-CA-C	-5.61	107.69	114.75
1	B	335	ILE	N-CA-C	-5.54	101.01	107.61
1	A	400	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	B	14	LEU	CA-C-N	-5.53	115.42	122.77
1	B	14	LEU	C-N-CA	-5.53	115.42	122.77
1	A	410	SER	N-CA-C	5.53	116.98	111.07
1	A	191	ILE	N-CA-C	-5.48	100.69	108.58
1	A	61	GLN	CB-CG-CD	5.43	121.84	112.60
1	A	274	SER	CA-CB-OG	-5.43	100.25	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	LEU	CB-CA-C	5.42	117.26	108.87
1	B	73	THR	CB-CA-C	5.41	118.11	109.62
1	B	157	THR	N-CA-C	-5.38	100.26	109.24
1	A	139	LEU	N-CA-C	5.36	117.54	111.11
1	B	61	GLN	CB-CA-C	-5.36	99.28	109.95
1	A	406	MET	CG-SD-CE	-5.32	89.20	100.90
1	A	52	HIS	CA-C-N	-5.32	112.23	120.31
1	A	52	HIS	C-N-CA	-5.32	112.23	120.31
1	A	33	THR	CB-CA-C	5.29	120.94	110.42
1	B	171	GLY	CA-C-O	-5.28	118.79	122.22
1	A	19	THR	N-CA-C	5.26	117.97	109.40
1	A	33	THR	CA-C-N	5.26	131.58	121.54
1	A	33	THR	C-N-CA	5.26	131.58	121.54
1	B	146	HIS	CA-C-N	5.21	124.82	119.56
1	B	146	HIS	C-N-CA	5.21	124.82	119.56
1	B	70	CYS	CA-CB-SG	-5.19	102.45	114.40
1	B	68	VAL	N-CA-C	5.15	116.49	110.62
1	A	370	LEU	CA-C-N	5.13	126.25	119.84
1	A	370	LEU	C-N-CA	5.13	126.25	119.84
1	A	338	VAL	N-CA-C	-5.09	102.29	109.21
1	A	409	PHE	CA-C-O	5.06	126.09	120.63
1	A	219	PHE	N-CA-C	-5.04	105.87	111.36
1	A	414	GLU	N-CA-C	5.00	117.47	111.71

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ASP	Peptide
1	A	33	THR	Peptide
1	A	370	LEU	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	3044	0	2980	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3047	0	2984	54	0
2	A	104	0	0	3	1
2	B	88	0	0	4	0
All	All	6283	0	5964	125	1

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 10.

All (125) 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:78:GLU:HG2	1:A:425:MET:HE1	1.27	1.10
1:A:78:GLU:HG2	1:A:425:MET:CE	1.88	1.03
1:A:316[A]:MET:CE	1:A:364:ILE:HD13	1.97	0.94
1:A:173:THR:HB	1:A:175:LYS:HE3	1.50	0.92
1:A:61:GLN:HE21	1:A:61:GLN:H	1.16	0.89
1:A:316[B]:MET:HE3	1:A:353:LEU:HD22	1.54	0.87
1:A:316[B]:MET:CE	1:A:353:LEU:HD22	2.04	0.86
1:A:175:LYS:HD3	1:A:175:LYS:H	1.42	0.85
1:B:285:VAL:HG23	1:B:316[A]:MET:HE3	1.62	0.82
1:B:182:GLU:HG3	1:B:225:PHE:CZ	2.15	0.81
1:A:32:HIS:HE1	1:A:404:TYR:OH	1.63	0.80
1:B:61:GLN:H	1:B:61:GLN:HE21	1.31	0.77
1:A:335:ILE:O	2:A:531:HOH:O	2.02	0.77
1:B:316[A]:MET:CE	1:B:379:LEU:HD12	2.15	0.76
1:A:316[A]:MET:HE3	1:A:364:ILE:HD13	1.66	0.76
1:B:32:HIS:HE1	1:B:404:TYR:OH	1.70	0.73
1:A:415:MET:HE2	1:A:420:ILE:HG12	1.71	0.72
1:A:316[A]:MET:CE	1:A:364:ILE:CD1	2.66	0.72
1:A:175:LYS:HD3	1:A:175:LYS:N	2.03	0.72
1:B:243:ILE:HG13	2:B:495:HOH:O	1.89	0.72
1:A:50:LYS:HE3	1:A:411:ASP:OD2	1.90	0.71
1:A:425:MET:O	1:A:425:MET:HE3	1.91	0.70
1:B:20:ASN:H	1:B:23:ASN:HD22	1.40	0.69
1:A:20:ASN:H	1:A:23:ASN:HD22	1.38	0.69
1:A:207:VAL:HA	1:A:210:HIS:HD2	1.59	0.68
1:A:316[A]:MET:HE1	1:A:364:ILE:HD13	1.76	0.67
1:B:319:GLY:HA2	1:B:364:ILE:HD11	1.75	0.67
1:A:35:THR:HG23	1:A:36:GLY:H	1.59	0.66
1:B:285:VAL:HG23	1:B:316[A]:MET:CE	2.24	0.66
1:B:32:HIS:HA	1:B:35:THR:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:THR:HG21	1:B:197:HIS:O	1.97	0.64
1:A:175:LYS:H	1:A:175:LYS:CD	2.11	0.63
1:B:182:GLU:HG3	1:B:225:PHE:HZ	1.62	0.62
1:A:78:GLU:CG	1:A:425:MET:CE	2.73	0.62
1:A:292:VAL:HG22	1:A:312:PHE:CE1	2.35	0.62
1:B:407:MET:HG2	1:B:411:ASP:HB2	1.81	0.62
1:A:50:LYS:HE3	1:A:411:ASP:CG	2.26	0.61
1:A:316[A]:MET:HE3	1:A:364:ILE:CD1	2.28	0.61
1:A:35:THR:HG23	1:A:36:GLY:N	2.14	0.61
1:B:128:VAL:O	1:B:146:HIS:HE1	1.83	0.60
1:A:135:ASN:ND2	1:A:138:GLU:H	2.00	0.60
1:A:286:ASN:OD1	1:A:317:ASN:ND2	2.35	0.60
1:A:78:GLU:HA	1:A:425:MET:HE2	1.82	0.60
1:B:316[A]:MET:HE2	1:B:379:LEU:HD12	1.82	0.60
1:B:286[B]:ASN:OD1	1:B:317:ASN:ND2	2.34	0.59
1:B:205:TYR:HB3	1:B:251:VAL:HG21	1.84	0.59
1:A:128:VAL:O	1:A:146:HIS:HE1	1.86	0.59
1:B:61:GLN:H	1:B:61:GLN:NE2	2.00	0.59
1:A:316[B]:MET:HE1	1:A:353:LEU:HD22	1.83	0.58
1:B:285:VAL:CG2	1:B:316[A]:MET:HE3	2.34	0.58
1:A:146:HIS:HD2	1:A:148:ASN:H	1.52	0.58
1:B:80:LEU:HB3	1:B:85:THR:HG21	1.86	0.57
1:B:20:ASN:C	1:B:20:ASN:HD22	2.12	0.57
1:A:61:GLN:H	1:A:61:GLN:NE2	1.97	0.57
1:B:32:HIS:HD2	1:B:38:ASN:O	1.88	0.57
1:A:328:LEU:HB3	1:B:361:LEU:HD11	1.86	0.57
1:B:53:SER:O	1:B:57:THR:HG23	2.05	0.56
1:A:35:THR:CG2	1:A:36:GLY:N	2.68	0.56
1:B:240:GLY:HA2	1:B:275:TYR:CD1	2.41	0.56
1:B:85:THR:HG23	1:B:86:GLY:O	2.07	0.55
1:A:320:VAL:HG21	1:A:328:LEU:CD1	2.37	0.55
1:A:32:HIS:HD2	1:A:38:ASN:O	1.90	0.54
1:B:99:GLN:HG3	2:B:470:HOH:O	2.07	0.53
1:A:238:PHE:HA	1:A:244:GLN:HE22	1.74	0.53
1:A:141:LYS:NZ	1:B:288:ILE:O	2.35	0.52
1:A:415:MET:HE2	1:A:420:ILE:CG1	2.40	0.51
1:B:109:ILE:HG12	1:B:130:ILE:CG2	2.41	0.51
1:B:406:MET:HE2	1:B:407:MET:N	2.26	0.51
1:A:351:SER:O	1:A:367:SER:HA	2.11	0.51
1:A:359:ASP:OD1	1:A:359:ASP:C	2.53	0.51
1:B:316[A]:MET:HE1	1:B:379:LEU:HD12	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:CA	1:A:425:MET:HE2	2.41	0.50
1:A:316[B]:MET:HE3	1:A:353:LEU:CD2	2.32	0.50
1:B:416:GLN:HG3	1:B:417:ASP:N	2.21	0.49
1:B:134:ASP:HB3	1:B:154:HIS:HB3	1.94	0.49
1:A:209:VAL:HG22	1:A:255:LEU:HD11	1.94	0.49
1:A:99:GLN:HE22	1:A:105:PRO:HD3	1.78	0.49
1:A:216:ARG:HG2	1:A:259:TYR:CD1	2.48	0.48
1:A:316[B]:MET:HE3	1:A:353:LEU:HB3	1.96	0.48
1:A:258:ILE:HG22	1:A:259:TYR:N	2.28	0.47
1:B:352:SER:HB3	1:B:366:GLU:O	2.14	0.47
1:B:19:THR:HG21	2:B:526:HOH:O	2.13	0.47
1:A:135:ASN:HD21	1:A:138:GLU:H	1.63	0.47
1:B:313:VAL:HG13	1:B:354:TRP:CD1	2.50	0.47
1:A:292:VAL:HG22	1:A:312:PHE:HE1	1.77	0.47
1:A:415:MET:CE	1:A:420:ILE:HD11	2.46	0.46
1:A:50:LYS:HE3	1:A:411:ASP:OD1	2.15	0.46
1:A:157:THR:HG21	1:A:197:HIS:O	2.16	0.46
1:B:146:HIS:HD2	1:B:148:ASN:H	1.62	0.46
1:A:131:MET:HE2	1:A:131:MET:HB3	1.66	0.46
1:A:322:GLY:CA	1:A:400:ARG:NH1	2.79	0.45
1:A:198:VAL:O	1:A:237:GLY:HA3	2.16	0.45
1:A:233:ASP:OD2	1:A:271:GLU:OE2	2.35	0.45
1:B:32:HIS:CE1	1:B:404:TYR:OH	2.59	0.45
1:B:233:ASP:OD2	1:B:271:GLU:OE2	2.34	0.45
1:A:316[B]:MET:CE	1:A:353:LEU:CD2	2.88	0.45
1:A:253:SER:HB3	1:A:254:PRO:HD3	1.99	0.45
1:A:320:VAL:HG21	1:A:328:LEU:HD11	1.98	0.44
1:B:182:GLU:HG3	1:B:225:PHE:CE1	2.52	0.44
1:A:242:GLU:OE1	2:A:546:HOH:O	2.21	0.44
1:A:78:GLU:HG2	1:A:425:MET:HE2	1.89	0.43
1:B:313:VAL:CG1	1:B:354:TRP:CD1	3.01	0.43
1:B:327:LYS:HE3	2:B:517:HOH:O	2.18	0.43
1:A:32:HIS:CE1	1:A:404:TYR:OH	2.56	0.43
1:A:313:VAL:HG13	1:A:354:TRP:CD1	2.54	0.43
1:B:277:VAL:O	1:B:278:SER:C	2.62	0.42
1:A:19:THR:CG2	2:A:540:HOH:O	2.66	0.42
1:A:134:ASP:HB3	1:A:154:HIS:HB3	2.01	0.42
1:B:349:PHE:CD2	1:B:349:PHE:N	2.88	0.42
1:B:59:VAL:HA	1:B:61:GLN:HE22	1.85	0.42
1:A:78:GLU:CB	1:A:425:MET:HE2	2.50	0.41
1:A:36:GLY:O	1:A:37:LYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:VAL:CG2	1:B:316[A]:MET:CE	2.95	0.41
1:B:15:LEU:CD1	1:B:406:MET:HE3	2.51	0.41
1:B:410:SER:O	1:B:414:GLU:HG3	2.20	0.41
1:A:31:GLU:O	1:A:35:THR:HB	2.21	0.41
1:A:277:VAL:O	1:A:385:GLY:HA3	2.21	0.41
1:B:20:ASN:ND2	1:B:23:ASN:H	2.19	0.41
1:B:47:LYS:O	1:B:51:LYS:HG2	2.20	0.41
1:B:406:MET:HE2	1:B:407:MET:CA	2.50	0.41
1:A:36:GLY:O	1:A:37:LYS:CB	2.68	0.41
1:A:91:SER:HB2	1:B:397:ASP:CG	2.45	0.40
1:A:427:LYS:NZ	1:A:428:ASN:HD21	2.18	0.40
1:B:131:MET:HE2	1:B:131:MET:HB3	2.00	0.40
1:B:110:PHE:CE2	1:B:115:LYS:HD3	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:550:HOH:O	2:A:550:HOH:O[2_665]	0.95	1.25

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	385/448 (86%)	364 (94%)	19 (5%)	2 (0%)	24	16
1	B	383/448 (86%)	373 (97%)	9 (2%)	1 (0%)	36	30
All	All	768/896 (86%)	737 (96%)	28 (4%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ALA
1	A	37	LYS
1	B	273	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	332/385 (86%)	311 (94%)	21 (6%)	16	9
1	B	336/385 (87%)	313 (93%)	23 (7%)	14	8
All	All	668/770 (87%)	624 (93%)	44 (7%)	15	9

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	33	THR
1	A	34	LEU
1	A	35	THR
1	A	61	GLN
1	A	109	ILE
1	A	157	THR
1	A	168	MET
1	A	175	LYS
1	A	200	SER
1	A	258	ILE
1	A	293	VAL
1	A	328	LEU
1	A	335	ILE
1	A	341	LYS
1	A	350	THR
1	A	359	ASP
1	A	406	MET
1	A	417	ASP
1	A	420	ILE
1	A	427	LYS

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Mol	Chain	Res	Type
1	B	17	GLU
1	B	20	ASN
1	B	33	THR
1	B	35	THR
1	B	61	GLN
1	B	85	THR
1	B	106	GLU
1	B	157	THR
1	B	175	LYS
1	B	186	GLU
1	B	204	GLU
1	B	206	GLN
1	B	291	LYS
1	B	334	THR
1	B	335	ILE
1	B	337	GLU
1	B	340	LYS
1	B	350	THR
1	B	351	SER
1	B	406	MET
1	B	416	GLN
1	B	417	ASP
1	B	434	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	32	HIS
1	A	56	GLN
1	A	61	GLN
1	A	99	GLN
1	A	135	ASN
1	A	146	HIS
1	A	154	HIS
1	A	210	HIS
1	A	244	GLN
1	A	249	ASN
1	A	339	HIS
1	A	374	ASN
1	A	399	GLN
1	A	428	ASN

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Mol	Chain	Res	Type
1	B	9	ASN
1	B	20	ASN
1	B	23	ASN
1	B	32	HIS
1	B	38	ASN
1	B	54	GLN
1	B	61	GLN
1	B	146	HIS
1	B	190	GLN
1	B	206	GLN
1	B	339	HIS
1	B	390	HIS
1	B	428	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	394/448 (87%)	0.15	33 (8%) 17 17	10, 25, 49, 59	2 (0%)
1	B	390/448 (87%)	0.22	25 (6%) 25 25	12, 27, 48, 58	3 (0%)
All	All	784/896 (87%)	0.18	58 (7%) 20 21	10, 26, 49, 59	5 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	TYR	6.7
1	B	347	PRO	6.6
1	B	311	ALA	5.4
1	A	347	PRO	4.7
1	B	34	LEU	4.0
1	A	293	VAL	3.6
1	B	36	GLY	3.5
1	B	335	ILE	3.5
1	B	8	ALA	3.4
1	B	292	VAL	3.4
1	B	395	PHE	3.4
1	B	417	ASP	3.3
1	A	36	GLY	3.3
1	A	335	ILE	3.2
1	B	349	PHE	3.2
1	B	348	LEU	3.1
1	B	358	CYS	3.1
1	A	334	THR	3.0
1	B	350	THR	3.0
1	A	18	GLY	3.0
1	A	203	LYS	2.9
1	A	341	LYS	2.9
1	A	435	CYS	2.9
1	A	358	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	430[A]	PHE	2.8
1	B	334	THR	2.7
1	A	292	VAL	2.6
1	A	205	TYR	2.6
1	B	18	GLY	2.5
1	A	202	CYS	2.5
1	A	413	TYR	2.5
1	A	8	ALA	2.5
1	B	17	GLU	2.5
1	A	417	ASP	2.4
1	A	201	ALA	2.4
1	A	159	ASP	2.4
1	B	35	THR	2.4
1	A	348	LEU	2.3
1	A	412	TRP	2.3
1	B	204	GLU	2.2
1	A	38	ASN	2.2
1	A	262	GLU	2.2
1	A	366	GLU	2.2
1	B	259	TYR	2.2
1	A	34	LEU	2.2
1	A	30	TYR	2.2
1	A	349	PHE	2.1
1	B	178	ARG	2.1
1	B	70	CYS	2.1
1	A	31	GLU	2.1
1	B	38	ASN	2.1
1	A	19	THR	2.1
1	A	224	GLU	2.1
1	B	159	ASP	2.1
1	A	35	THR	2.1
1	A	420	ILE	2.1
1	B	168	MET	2.0
1	A	188	ASP	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.