Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 10:11 PM EDT

PDB ID	:	3BTN
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 (i) 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 (1)) were used in the production of this report:

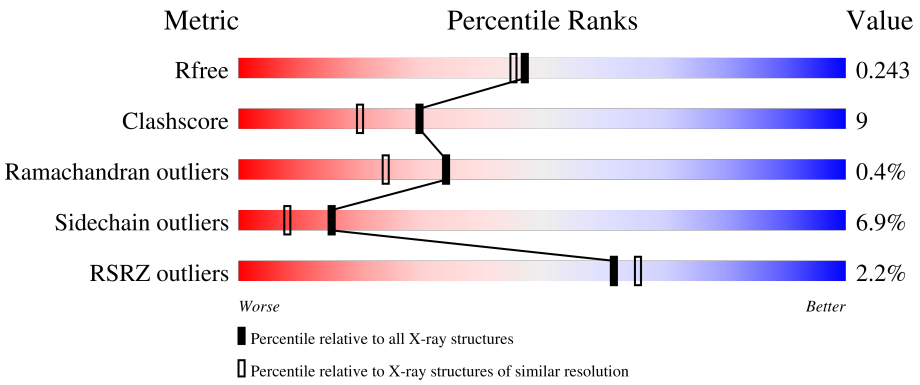
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.05 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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 <=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	2% 62% 20% 6% 12%
1	B	448	2% 64% 20% • • 13%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	394	3044	1964	486	569	25	0	1	0
1	B	390	3047	1965	484	574	24	0	3	0

- Molecule 2 is water.

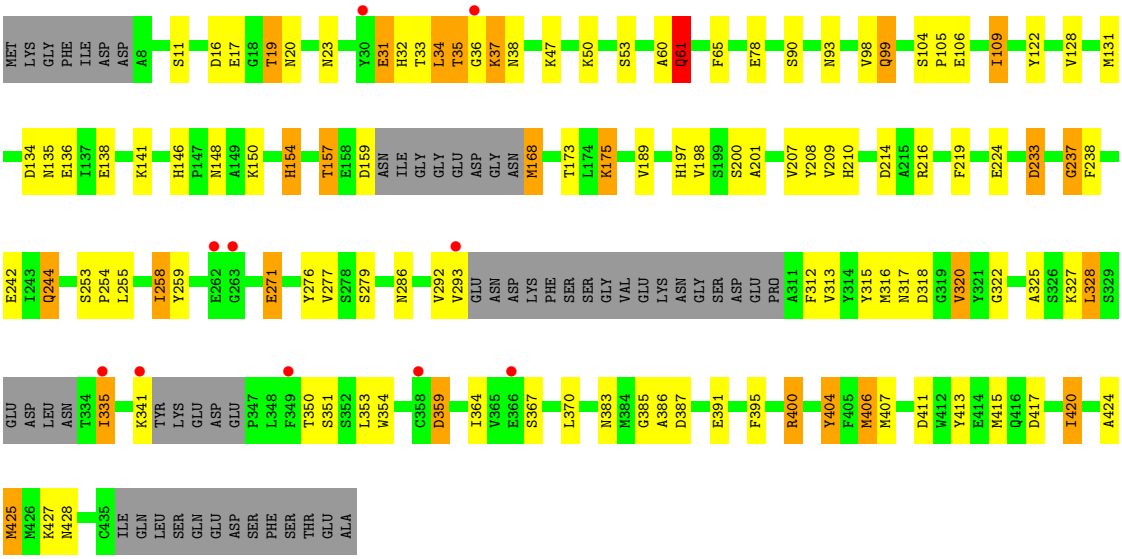
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	104	104	104	0	0
2	B	88	88	88	0	0

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.

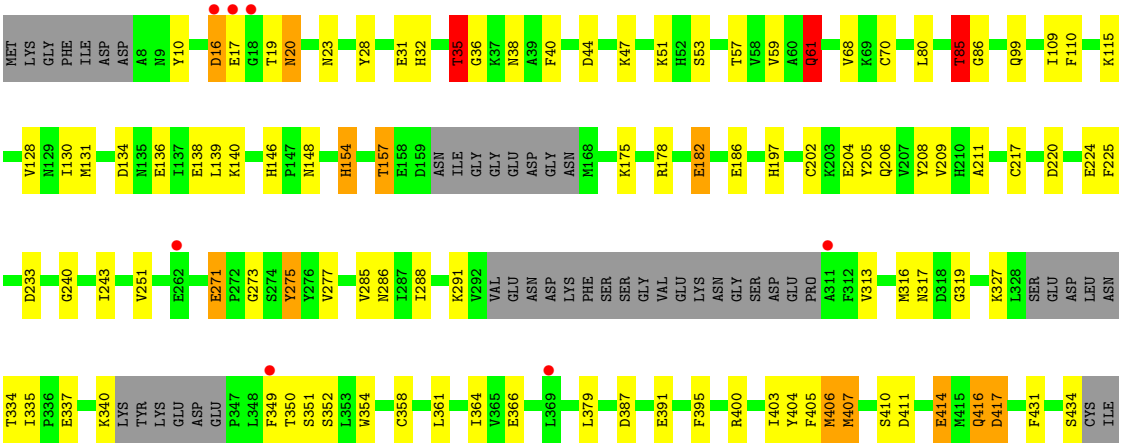
• Molecule 1: Antizyme inhibitor 1

Chain A:



• Molecule 1: Antizyme inhibitor 1

Chain B:



GLN
LEU
SER
GLN
GLU
ASP
SER
PHE
SER
THR
GLU
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 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 49.58 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.05) 99.8 (49.58-2.04)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.83 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.241 0.198 , 0.243	Depositor DCC
R_{free} test set	3477 reflections (5.06%)	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 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	1.67	36/3115 (1.2%)	1.26	16/4217 (0.4%)
1	B	1.62	32/3125 (1.0%)	1.23	16/4230 (0.4%)
All	All	1.64	68/6240 (1.1%)	1.25	32/8447 (0.4%)

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 (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	TYR	CD1-CE1	8.95	1.52	1.39
1	B	387	ASP	CB-CG	8.93	1.70	1.51
1	A	320	VAL	CB-CG2	-8.13	1.35	1.52
1	B	178	ARG	CG-CD	7.98	1.71	1.51
1	B	208	TYR	CD2-CE2	7.88	1.51	1.39
1	B	209	VAL	CB-CG1	7.81	1.69	1.52
1	A	391	GLU	CG-CD	7.58	1.63	1.51
1	A	106	GLU	CB-CG	7.43	1.66	1.52
1	B	414	GLU	CG-CD	7.38	1.63	1.51
1	B	358	CYS	CB-SG	7.37	1.94	1.82
1	B	391	GLU	CD-OE2	7.37	1.33	1.25
1	B	391	GLU	CG-CD	7.09	1.62	1.51
1	B	10	TYR	CD2-CE2	6.98	1.49	1.39
1	B	31	GLU	CG-CD	6.91	1.62	1.51
1	B	275	TYR	CD2-CE2	6.89	1.49	1.39
1	B	271	GLU	CG-CD	6.88	1.62	1.51
1	A	136	GLU	CG-CD	6.85	1.62	1.51
1	A	315	TYR	CD1-CE1	6.85	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	GLU	CG-CD	6.66	1.61	1.51
1	B	68	VAL	CB-CG1	6.58	1.66	1.52
1	A	400	ARG	CZ-NH2	6.55	1.41	1.33
1	A	31	GLU	CG-CD	6.50	1.61	1.51
1	B	403	ILE	CB-CG2	6.47	1.73	1.52
1	A	104	SER	CB-OG	-6.41	1.33	1.42
1	A	90	SER	CB-OG	-6.38	1.33	1.42
1	A	404	TYR	CD1-CE1	6.30	1.48	1.39
1	B	202	CYS	CB-SG	6.27	1.93	1.82
1	A	11	SER	CB-OG	-6.25	1.34	1.42
1	B	224	GLU	CG-CD	6.12	1.61	1.51
1	A	276	TYR	CD1-CE1	6.07	1.48	1.39
1	A	271	GLU	CG-CD	6.05	1.61	1.51
1	A	98	VAL	CB-CG1	-6.01	1.40	1.52
1	A	60	ALA	CA-CB	5.98	1.65	1.52
1	B	224	GLU	CB-CG	5.97	1.63	1.52
1	A	189	VAL	CB-CG1	5.93	1.65	1.52
1	B	277	VAL	CB-CG1	5.87	1.65	1.52
1	B	136	GLU	CG-CD	5.85	1.60	1.51
1	A	386	ALA	CA-CB	5.82	1.64	1.52
1	A	413	TYR	CD2-CE2	5.82	1.48	1.39
1	B	395	PHE	CE1-CZ	5.75	1.48	1.37
1	A	395	PHE	CE1-CZ	5.72	1.48	1.37
1	A	383	ASN	CB-CG	5.62	1.64	1.51
1	B	138	GLU	CG-CD	5.56	1.60	1.51
1	B	208	TYR	CD1-CE1	5.53	1.47	1.39
1	B	28	TYR	CD2-CE2	-5.48	1.31	1.39
1	B	217	CYS	CB-SG	5.48	1.91	1.82
1	B	140	LYS	CE-NZ	5.45	1.62	1.49
1	B	431	PHE	CE2-CZ	5.42	1.47	1.37
1	A	31	GLU	CD-OE2	5.42	1.31	1.25
1	B	405	PHE	CD2-CE2	5.32	1.49	1.39
1	A	325	ALA	CA-CB	5.32	1.63	1.52
1	B	40	PHE	CE2-CZ	5.30	1.47	1.37
1	A	279	SER	CA-CB	5.25	1.60	1.52
1	A	65	PHE	CE1-CZ	5.25	1.47	1.37
1	A	424	ALA	CA-CB	5.25	1.63	1.52
1	A	391	GLU	CD-OE2	5.25	1.31	1.25
1	B	31	GLU	CB-CG	5.24	1.62	1.52
1	A	61	GLN	CG-CD	5.21	1.63	1.51
1	A	219	PHE	CD1-CE1	5.21	1.49	1.39
1	A	224	GLU	CG-CD	5.21	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	44	ASP	CB-CG	5.20	1.62	1.51
1	A	99	GLN	CG-CD	5.19	1.62	1.51
1	A	208	TYR	CE2-CZ	5.12	1.45	1.38
1	A	237	GLY	N-CA	5.05	1.53	1.46
1	B	211	ALA	CA-CB	5.04	1.63	1.52
1	A	93	ASN	CB-CG	5.03	1.62	1.51
1	A	387	ASP	CB-CG	5.02	1.62	1.51
1	A	53	SER	CB-OG	-5.01	1.35	1.42

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	178	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	B	178	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	A	407	MET	CA-CB-CG	10.16	130.57	113.30
1	A	34	LEU	N-CA-C	-10.02	83.96	111.00
1	B	220	ASP	CB-CG-OD1	9.54	126.89	118.30
1	A	17	GLU	N-CA-C	-9.47	85.42	111.00
1	A	400	ARG	NE-CZ-NH1	-8.67	115.96	120.30
1	B	131	MET	CA-CB-CG	7.69	126.38	113.30
1	A	318	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	B	400	ARG	NE-CZ-NH1	-7.15	116.73	120.30
1	B	406	MET	CG-SD-CE	6.90	111.25	100.20
1	A	406	MET	CG-SD-CE	-6.88	89.20	100.20
1	A	233	ASP	CB-CG-OD1	6.87	124.48	118.30
1	B	139	LEU	CB-CG-CD2	-6.68	99.64	111.00
1	B	70	CYS	CA-CB-SG	-6.41	102.45	114.00
1	A	233	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	B	85	THR	OG1-CB-CG2	6.29	124.46	110.00
1	A	131	MET	CA-CB-CG	5.84	123.23	113.30
1	A	168	MET	CG-SD-CE	5.79	109.47	100.20
1	A	425	MET	CG-SD-CE	-5.71	91.06	100.20
1	A	109	ILE	CB-CG1-CD1	-5.71	97.92	113.90
1	A	150	LYS	CD-CE-NZ	-5.60	98.81	111.70
1	B	407	MET	CA-CB-CG	5.60	122.81	113.30
1	B	36	GLY	N-CA-C	5.57	127.03	113.10
1	B	61	GLN	CB-CA-C	-5.56	99.28	110.40
1	A	99	GLN	CA-CB-CG	5.47	125.43	113.40
1	B	35	THR	N-CA-C	-5.45	96.28	111.00
1	A	214	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	387	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	220	ASP	CB-CG-OD2	-5.16	113.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	16	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	159	ASP	CB-CG-OD1	5.09	122.88	118.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3044	0	2980	66	0
1	B	3047	0	2984	49	0
2	A	104	0	0	3	1
2	B	88	0	0	5	0
All	All	6283	0	5964	113	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 9.

All (113) 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	1.18	1.16
1:A:78:GLU:HG2	1:A:425:MET:CE	1.88	1.03
1:A:316[B]:MET:HE3	1:A:353:LEU:HD22	1.45	0.96
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:CE	1:A:353:LEU:HD22	2.04	0.86
1:A:175:LYS:HD3	1:A:175:LYS:H	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316[A]:MET:HE3	1:A:364:ILE:HD13	1.61	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:285:VAL:HG23	1:B:316[A]:MET:HE3	1.65	0.79
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:78:GLU:CG	1:A:425:MET:HE1	2.10	0.75
1:B:32:HIS:HE1	1:B:404:TYR:OH	1.70	0.73
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: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: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:316[A]:MET:HE1	1:B:379:LEU:HD12	1.77	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
1:B:157:THR:HG21	1:B:197:HIS:O	1.97	0.64
1:A:316[A]:MET:HE3	1:A:364:ILE:CD1	2.27	0.63
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: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:316[A]:MET:HE1	1:A:364:ILE:HD13	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:316[B]:MET:HE3	1:A:353:LEU:CD2	2.26	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: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:A:61:GLN:H	1:A:61:GLN:NE2	1.97	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:HIS:HD2	1:B:38:ASN:O	1.88	0.57
1:A:50:LYS:HE3	1:A:411:ASP:CG	2.26	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:B:20:ASN:C	1:B:20:ASN:HD22	2.12	0.52
1:B:109:ILE:HG12	1:B:130:ILE:CG2	2.41	0.51
1:A:351:SER:O	1:A:367:SER:HA	2.11	0.51
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:B:285:VAL:CG2	1:B:316[A]:MET:HE3	2.40	0.48
1:A:258:ILE:HG22	1:A:259:TYR:N	2.28	0.47
1:A:316[B]:MET:HE1	1:A:353:LEU:HD22	1.93	0.47
1:B:316[A]:MET:HE2	1:B:379:LEU:HD12	1.95	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:B:327:LYS:NZ	2:B:517:HOH:O	2.47	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:A:359:ASP:OD1	1:A:359:ASP:C	2.53	0.46
1:B:146:HIS:HD2	1:B:148:ASN:H	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:NZ	1:B:288:ILE:O	2.35	0.44
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: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: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:36:GLY:O	1:A:37:LYS:HB3	2.20	0.41
1:B:285:VAL:CG2	1:B:316[A]:MET:CE	2.95	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:A:36:GLY:O	1:A:37:LYS:CB	2.68	0.41
1:A:427:LYS:NZ	1:A:428:ASN:HD21	2.18	0.40
1:A:316[B]:MET:HE3	1:A:353:LEU:HB3	2.04	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%)	29	18
1	B	383/448 (86%)	373 (97%)	9 (2%)	1 (0%)	41	31
All	All	768/896 (86%)	737 (96%)	28 (4%)	3 (0%)	34	24

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%)	309 (93%)	23 (7%)	15	8
1	B	336/385 (87%)	313 (93%)	23 (7%)	16	8
All	All	668/770 (87%)	622 (93%)	46 (7%)	15	8

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	34	LEU
1	A	35	THR
1	A	47	LYS
1	A	61	GLN
1	A	109	ILE
1	A	154	HIS
1	A	157	THR
1	A	168	MET
1	A	175	LYS
1	A	200	SER
1	A	244	GLN
1	A	258	ILE

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Mol	Chain	Res	Type
1	A	293	VAL
1	A	327	LYS
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	B	16	ASP
1	B	17	GLU
1	B	20	ASN
1	B	35	THR
1	B	61	GLN
1	B	85	THR
1	B	154	HIS
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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	32	HIS
1	A	54	GLN
1	A	61	GLN
1	A	99	GLN

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Mol	Chain	Res	Type
1	A	135	ASN
1	A	146	HIS
1	A	210	HIS
1	A	244	GLN
1	A	339	HIS
1	A	390	HIS
1	A	428	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	339	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 monosaccharides 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 (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	394/448 (87%)	-0.10	10 (2%)	57	61	10, 25, 49, 59	1 (0%)
1	B	390/448 (87%)	-0.13	7 (1%)	68	71	13, 27, 48, 58	0
All	All	784/896 (87%)	-0.11	17 (2%)	62	66	10, 26, 49, 59	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	ILE	5.3
1	A	293	VAL	4.0
1	A	262	GLU	3.1
1	B	311	ALA	2.9
1	A	341	LYS	2.8
1	B	349	PHE	2.6
1	A	263	GLY	2.5
1	B	18	GLY	2.5
1	B	16	ASP	2.4
1	B	262	GLU	2.3
1	A	349	PHE	2.3
1	A	366	GLU	2.3
1	A	36	GLY	2.2
1	A	358	CYS	2.1
1	B	17	GLU	2.1
1	A	30	TYR	2.1
1	B	369	LEU	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 monosaccharides 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.