Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:38 pm BST

PDB ID	:	1AGX
Title	:	REFINED CRYSTAL STRUCTURE OF ACINETOBACTER GLUTAMINASIFICANS GLUTAMINASE-ASPARAGINASE
Authors	:	Lubkowski, J.; Wlodawer, A.; Housset, D.; Weber, I.T.; Ammon, H.L.; Murphy, K.C.; Swain, A.L.
Deposited on	:	1994-07-13
Resolution	:	2.90 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 following versions of software and data (see references ①) were used in the production of this report:

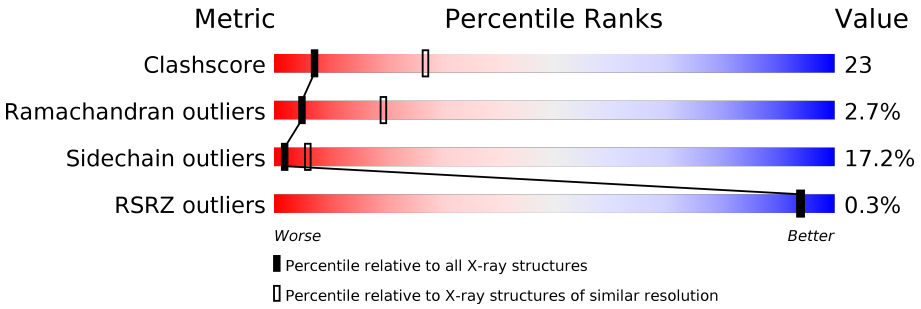
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	331	45% 37% 14% ·

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2497 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 GLUTAMINASE-ASPARAGINASE.

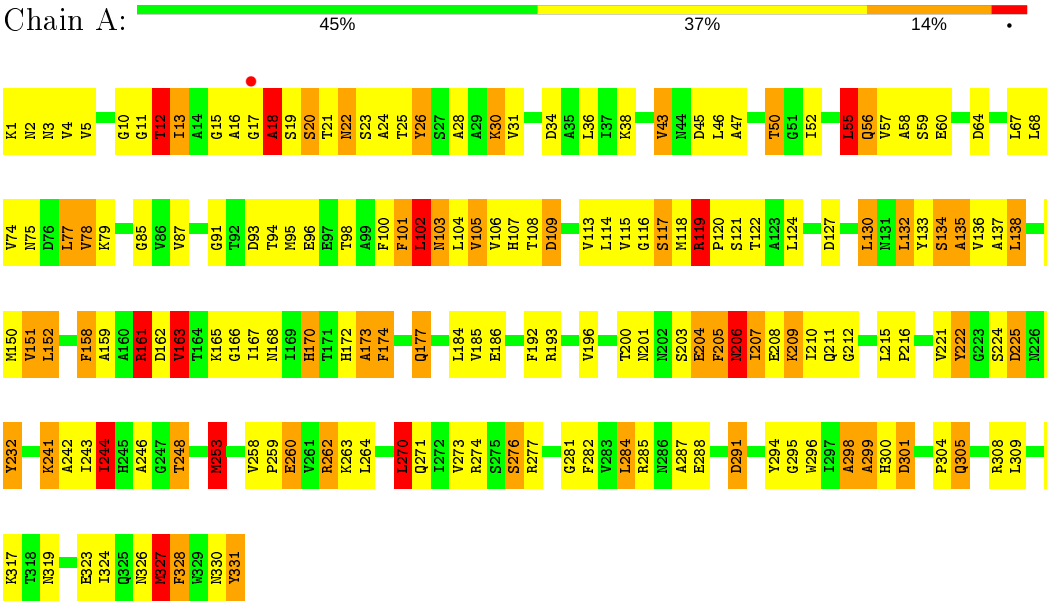
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	2497	1573	437	478	9	0	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: GLUTAMINASE-ASPARAGINASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	96.60Å 112.50Å 71.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 9.99 – 2.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.90) 84.1 (9.99-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.171 , (Not available) 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 55.5	EDS
L-test for twinning[1]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2497	wwPDB-VP
Average B, all atoms (Å^2)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] 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

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	1.07	0/2541	2.25	109/3451 (3.2%)

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

There are no bond length outliers.

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	ARG	NE-CZ-NH2	-19.93	110.34	120.30
1	A	26	TYR	CA-CB-CG	18.36	148.29	113.40
1	A	93	ASP	CB-CG-OD1	15.39	132.15	118.30
1	A	161	ARG	NE-CZ-NH1	15.00	127.80	120.30
1	A	277	ARG	NE-CZ-NH1	14.88	127.74	120.30
1	A	87	VAL	CA-CB-CG1	12.57	129.76	110.90
1	A	158	PHE	CB-CG-CD1	-12.57	112.00	120.80
1	A	205	PHE	CB-CG-CD2	-12.14	112.31	120.80
1	A	127	ASP	CB-CG-OD1	11.42	128.58	118.30
1	A	225	ASP	CB-CA-C	11.29	132.99	110.40
1	A	161	ARG	NH1-CZ-NH2	-10.72	107.61	119.40
1	A	109	ASP	CB-CG-OD1	10.47	127.72	118.30
1	A	56	GLN	N-CA-CB	10.07	128.73	110.60
1	A	274	ARG	NE-CZ-NH2	10.05	125.33	120.30
1	A	93	ASP	CB-CG-OD2	-9.96	109.34	118.30
1	A	161	ARG	CD-NE-CZ	9.86	137.41	123.60
1	A	294	TYR	CB-CG-CD2	-9.71	115.17	121.00
1	A	101	PHE	CB-CG-CD1	-9.64	114.05	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	LEU	CA-CB-CG	9.45	137.03	115.30
1	A	55	LEU	CA-CB-CG	9.04	136.10	115.30
1	A	26	TYR	CB-CG-CD2	8.76	126.26	121.00
1	A	291	ASP	O-C-N	8.73	136.67	122.70
1	A	87	VAL	CG1-CB-CG2	-8.72	96.95	110.90
1	A	105	VAL	CA-CB-CG2	-8.69	97.87	110.90
1	A	30	LYS	N-CA-C	8.56	134.12	111.00
1	A	205	PHE	CB-CG-CD1	8.53	126.77	120.80
1	A	45	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	119	ARG	CD-NE-CZ	8.20	135.08	123.60
1	A	151	VAL	CA-CB-CG1	7.83	122.64	110.90
1	A	244	ILE	CB-CA-C	7.80	127.19	111.60
1	A	317	LYS	CA-CB-CG	7.74	130.42	113.40
1	A	270	LEU	CA-CB-CG	7.61	132.79	115.30
1	A	158	PHE	CB-CG-CD2	7.50	126.05	120.80
1	A	101	PHE	CB-CG-CD2	7.43	126.00	120.80
1	A	308	ARG	N-CA-CB	7.38	123.88	110.60
1	A	262	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	A	222	TYR	CB-CG-CD2	7.37	125.42	121.00
1	A	22	ASN	C-N-CA	7.30	139.95	121.70
1	A	294	TYR	CB-CG-CD1	7.28	125.37	121.00
1	A	102	LEU	C-N-CA	7.23	139.76	121.70
1	A	161	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	A	253	MET	O-C-N	6.90	133.74	122.70
1	A	291	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	A	96	GLU	CA-CB-CG	6.77	128.29	113.40
1	A	174	PHE	O-C-N	6.75	133.50	122.70
1	A	328	PHE	CB-CG-CD1	6.67	125.47	120.80
1	A	68	LEU	CB-CA-C	6.66	122.86	110.20
1	A	309	LEU	CB-CG-CD1	-6.48	99.99	111.00
1	A	56	GLN	CB-CG-CD	6.46	128.38	111.60
1	A	158	PHE	CD1-CE1-CZ	6.45	127.84	120.10
1	A	193	ARG	CD-NE-CZ	6.43	132.61	123.60
1	A	173	ALA	N-CA-CB	-6.42	101.11	110.10
1	A	103	ASN	CA-C-N	-6.39	103.13	117.20
1	A	298	ALA	N-CA-CB	6.30	118.93	110.10
1	A	225	ASP	C-N-CA	6.29	137.43	121.70
1	A	109	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	A	260	GLU	OE1-CD-OE2	6.23	130.78	123.30
1	A	170	HIS	N-CA-CB	-6.18	99.48	110.60
1	A	165	LYS	CA-CB-CG	-6.16	99.86	113.40
1	A	166	GLY	CA-C-O	-6.01	109.79	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	193	ARG	CB-CG-CD	5.97	127.13	111.60
1	A	277	ARG	CG-CD-NE	5.93	124.26	111.80
1	A	165	LYS	CB-CA-C	5.90	122.20	110.40
1	A	276	SER	N-CA-CB	5.89	119.33	110.50
1	A	248	THR	CA-CB-CG2	5.86	120.61	112.40
1	A	331	TYR	N-CA-C	5.84	126.77	111.00
1	A	102	LEU	CB-CG-CD2	-5.82	101.11	111.00
1	A	135	ALA	CB-CA-C	5.80	118.80	110.10
1	A	244	ILE	CA-C-O	5.75	132.18	120.10
1	A	87	VAL	O-C-N	5.74	131.89	122.70
1	A	196	VAL	CB-CA-C	5.72	122.26	111.40
1	A	173	ALA	CB-CA-C	5.68	118.63	110.10
1	A	206	ASN	CA-C-N	5.62	129.56	117.20
1	A	323	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	A	43	VAL	CB-CA-C	5.60	122.04	111.40
1	A	288	GLU	CA-CB-CG	5.57	125.66	113.40
1	A	327	MET	CA-CB-CG	-5.57	103.82	113.30
1	A	114	LEU	N-CA-C	-5.53	96.07	111.00
1	A	274	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	A	328	PHE	CB-CG-CD2	-5.50	116.95	120.80
1	A	323	GLU	N-CA-CB	5.50	120.49	110.60
1	A	163	VAL	CA-CB-CG2	5.40	119.00	110.90
1	A	158	PHE	CG-CD1-CE1	-5.39	114.87	120.80
1	A	316	THR	N-CA-CB	5.38	120.53	110.30
1	A	68	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	204	GLU	CG-CD-OE2	-5.35	107.61	118.30
1	A	167	ILE	O-C-N	-5.29	114.23	122.70
1	A	225	ASP	O-C-N	-5.24	114.32	122.70
1	A	87	VAL	CA-CB-CG2	-5.22	103.07	110.90
1	A	192	PHE	CD1-CG-CD2	5.22	125.08	118.30
1	A	151	VAL	CA-C-N	-5.18	105.81	117.20
1	A	60	GLU	CA-CB-CG	5.17	124.77	113.40
1	A	106	VAL	CA-CB-CG2	5.16	118.64	110.90
1	A	232	TYR	CB-CG-CD2	5.16	124.09	121.00
1	A	64	ASP	CA-CB-CG	5.15	124.74	113.40
1	A	168	ASN	N-CA-C	5.13	124.86	111.00
1	A	185	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	A	323	GLU	CB-CG-CD	5.10	127.96	114.20
1	A	127	ASP	OD1-CG-OD2	-5.09	113.63	123.30
1	A	117	SER	N-CA-CB	-5.06	102.90	110.50
1	A	148	GLY	N-CA-C	-5.05	100.47	113.10
1	A	93	ASP	O-C-N	5.04	130.76	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	LEU	CB-CG-CD1	5.04	119.56	111.00
1	A	284	LEU	CA-CB-CG	5.04	126.88	115.30
1	A	138	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	330	ASN	N-CA-C	5.03	124.57	111.00
1	A	291	ASP	CA-CB-CG	-5.02	102.35	113.40
1	A	18	ALA	N-CA-CB	5.01	117.12	110.10
1	A	96	GLU	C-N-CA	5.01	134.24	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	ARG	Sidechain
1	A	161	ARG	Sidechain

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	2497	0	2514	113	0
All	All	2497	0	2514	113	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 23.

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:305:GLN:H	1:A:305:GLN:NE2	1.65	0.94
1:A:15:GLY:HA2	1:A:31:VAL:HG23	1.48	0.93
1:A:22:ASN:ND2	1:A:23:SER:H	1.72	0.87
1:A:305:GLN:H	1:A:305:GLN:HE21	1.18	0.87
1:A:16:ALA:HB2	1:A:121:SER:H	1.41	0.85
1:A:22:ASN:HD22	1:A:23:SER:H	1.24	0.85
1:A:242:ALA:HB2	1:A:271:GLN:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:PHE:O	1:A:105:VAL:HG22	1.85	0.77
1:A:244:ILE:HD11	1:A:304:PRO:HB3	1.66	0.76
1:A:159:ALA:O	1:A:163:VAL:HG12	1.87	0.74
1:A:264:LEU:O	1:A:270:LEU:HB2	1.93	0.69
1:A:59:SER:HB2	1:A:91:GLY:HA3	1.75	0.69
1:A:16:ALA:HB2	1:A:121:SER:N	2.07	0.68
1:A:78:VAL:HG21	1:A:108:THR:HG21	1.74	0.68
1:A:222:TYR:HA	1:A:246:ALA:HB3	1.78	0.66
1:A:118:MET:CE	1:A:173:ALA:HB3	2.26	0.66
1:A:170:HIS:HB3	1:A:172:HIS:ND1	2.10	0.66
1:A:52:ILE:HD12	1:A:77:LEU:HD21	1.79	0.64
1:A:12:THR:HG22	1:A:120:PRO:HA	1.78	0.64
1:A:177:GLN:HE22	1:A:281:GLY:H	1.47	0.63
1:A:20:SER:HA	1:A:122:THR:O	1.98	0.63
1:A:170:HIS:HB3	1:A:172:HIS:CE1	2.34	0.62
1:A:4:VAL:HA	1:A:85:GLY:O	2.00	0.62
1:A:43:VAL:HG23	1:A:133:TYR:HA	1.82	0.62
1:A:243:ILE:HG12	1:A:270:LEU:HD12	1.84	0.60
1:A:118:MET:HE1	1:A:173:ALA:HB3	1.82	0.60
1:A:10:GLY:HA2	1:A:56:GLN:NE2	2.17	0.60
1:A:59:SER:OG	1:A:94:THR:HB	2.02	0.60
1:A:2:ASN:O	1:A:47:ALA:HB1	2.01	0.59
1:A:273:VAL:CG1	1:A:299:ALA:HB2	2.33	0.59
1:A:253:MET:HG2	1:A:258:VAL:HG23	1.85	0.58
1:A:17:GLY:HA2	1:A:30:LYS:HD2	1.84	0.58
1:A:16:ALA:CB	1:A:121:SER:OG	2.52	0.57
1:A:57:VAL:HG12	1:A:58:ALA:N	2.19	0.57
1:A:151:VAL:HG22	1:A:158:PHE:CD2	2.39	0.57
1:A:98:THR:HG22	1:A:102:LEU:HD22	1.87	0.57
1:A:70:LEU:O	1:A:74:VAL:HG23	2.05	0.56
1:A:151:VAL:HG13	1:A:163:VAL:HG11	1.88	0.56
1:A:242:ALA:CB	1:A:271:GLN:HB2	2.36	0.56
1:A:282:PHE:HB3	1:A:301:ASP:HB3	1.88	0.56
1:A:95:MET:HE1	1:A:116:GLY:HA3	1.87	0.56
1:A:132:LEU:O	1:A:136:VAL:HG23	2.06	0.56
1:A:327:MET:O	1:A:331:TYR:HD2	1.88	0.56
1:A:16:ALA:HB3	1:A:121:SER:OG	2.06	0.55
1:A:10:GLY:HA2	1:A:56:GLN:OE1	2.07	0.55
1:A:107:HIS:CE1	1:A:203:SER:O	2.60	0.55
1:A:17:GLY:CA	1:A:30:LYS:HD2	2.37	0.54
1:A:130:LEU:O	1:A:134:SER:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLY:HA2	1:A:56:GLN:CD	2.28	0.53
1:A:100:PHE:O	1:A:103:ASN:HB3	2.10	0.52
1:A:221:VAL:HG11	1:A:232:TYR:CZ	2.46	0.51
1:A:13:ILE:HB	1:A:117:SER:HB2	1.92	0.51
1:A:18:ALA:HB3	1:A:25:THR:HB	1.92	0.51
1:A:107:HIS:HE1	1:A:203:SER:O	1.93	0.51
1:A:94:THR:CG2	1:A:94:THR:O	2.59	0.50
1:A:138:LEU:HD22	1:A:152:LEU:HD23	1.94	0.50
1:A:205:PHE:HA	1:A:209:LYS:HE3	1.93	0.50
1:A:107:HIS:HE1	1:A:205:PHE:O	1.93	0.49
1:A:305:GLN:N	1:A:305:GLN:HE21	1.99	0.49
1:A:109:ASP:HB3	1:A:201:ASN:HD21	1.77	0.49
1:A:13:ILE:HB	1:A:117:SER:CB	2.43	0.49
1:A:206:ASN:HD22	1:A:206:ASN:C	2.14	0.49
1:A:291:ASP:O	1:A:295:GLY:N	2.46	0.49
1:A:15:GLY:HA2	1:A:31:VAL:H	1.78	0.49
1:A:285:ARG:HA	1:A:298:ALA:HB2	1.94	0.48
1:A:258:VAL:HG22	1:A:296:TRP:HH2	1.78	0.48
1:A:241:LYS:HB3	1:A:315:LEU:HD13	1.95	0.48
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.63	0.48
1:A:57:VAL:HG12	1:A:58:ALA:O	2.13	0.47
1:A:215:LEU:HB3	1:A:216:PRO:HD2	1.95	0.47
1:A:151:VAL:O	1:A:158:PHE:N	2.26	0.46
1:A:105:VAL:H	1:A:105:VAL:HG22	1.44	0.46
1:A:18:ALA:HB3	1:A:25:THR:CB	2.46	0.46
1:A:75:ASN:O	1:A:79:LYS:HG3	2.16	0.46
1:A:15:GLY:CA	1:A:31:VAL:HG23	2.33	0.45
1:A:177:GLN:NE2	1:A:281:GLY:H	2.11	0.45
1:A:67:LEU:HA	1:A:67:LEU:HD23	1.70	0.45
1:A:324:ILE:HG22	1:A:328:PHE:HE2	1.82	0.45
1:A:15:GLY:HA2	1:A:31:VAL:N	2.31	0.45
1:A:46:LEU:HD13	1:A:137:ALA:HB2	1.98	0.45
1:A:207:ILE:N	1:A:207:ILE:HD12	2.32	0.45
1:A:324:ILE:HG22	1:A:328:PHE:CE2	2.51	0.45
1:A:55:LEU:HB3	1:A:57:VAL:HG23	1.99	0.45
1:A:16:ALA:HB2	1:A:121:SER:OG	2.17	0.45
1:A:13:ILE:C	1:A:15:GLY:H	2.21	0.45
1:A:161:ARG:HB2	1:A:161:ARG:HE	1.24	0.44
1:A:1:LYS:HA	1:A:1:LYS:HD3	1.76	0.44
1:A:151:VAL:HG22	1:A:158:PHE:HD2	1.82	0.44
1:A:5:VAL:HG13	1:A:50:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:HD11	1:A:304:PRO:CB	2.44	0.44
1:A:207:ILE:HA	1:A:210:ILE:HD12	2.00	0.43
1:A:12:THR:HA	1:A:15:GLY:O	2.18	0.43
1:A:13:ILE:HG13	1:A:36:LEU:HD11	1.99	0.43
1:A:203:SER:O	1:A:204:GLU:C	2.57	0.43
1:A:101:PHE:CE1	1:A:313:LEU:HD21	2.53	0.43
1:A:107:HIS:CE1	1:A:205:PHE:O	2.71	0.43
1:A:13:ILE:HD12	1:A:13:ILE:O	2.19	0.43
1:A:104:LEU:HD23	1:A:313:LEU:CD1	2.49	0.43
1:A:77:LEU:HA	1:A:77:LEU:HD12	1.88	0.43
1:A:69:SER:O	1:A:73:GLN:HG3	2.19	0.42
1:A:224:SER:O	1:A:227:MET:HG3	2.19	0.42
1:A:163:VAL:CG2	1:A:174:PHE:HD2	2.32	0.42
1:A:57:VAL:CG1	1:A:58:ALA:N	2.82	0.42
1:A:101:PHE:CE1	1:A:313:LEU:HD11	2.55	0.42
1:A:118:MET:HE3	1:A:173:ALA:HB3	2.00	0.42
1:A:229:PRO:HB3	1:A:260:GLU:HG2	2.02	0.41
1:A:113:VAL:HA	1:A:150:MET:O	2.21	0.41
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.89	0.41
1:A:79:LYS:CE	1:A:208:GLU:OE2	2.69	0.41
1:A:258:VAL:HG13	1:A:262:ARG:HG3	2.02	0.41
1:A:282:PHE:HB2	1:A:300:HIS:C	2.42	0.41
1:A:170:HIS:CB	1:A:172:HIS:CE1	3.04	0.40
1:A:115:VAL:HG21	1:A:135:ALA:HB2	2.04	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	329/331 (99%)	289 (88%)	31 (9%)	9 (3%)	5 19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	18	ALA
1	A	200	THR
1	A	212	GLY
1	A	287	ALA
1	A	11	GLY
1	A	28	ALA
1	A	24	ALA
1	A	299	ALA

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	267/267 (100%)	221 (83%)	46 (17%)	2 6

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

Mol	Chain	Res	Type
1	A	3	ASN
1	A	12	THR
1	A	13	ILE
1	A	19	SER
1	A	20	SER
1	A	21	THR
1	A	26	TYR
1	A	34	ASP
1	A	38	LYS
1	A	50	THR
1	A	55	LEU
1	A	77	LEU
1	A	78	VAL
1	A	102	LEU
1	A	119	ARG
1	A	124	LEU

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Mol	Chain	Res	Type
1	A	130	LEU
1	A	132	LEU
1	A	134	SER
1	A	142	ASN
1	A	152	LEU
1	A	161	ARG
1	A	162	ASP
1	A	163	VAL
1	A	177	GLN
1	A	184	LEU
1	A	186	GLU
1	A	206	ASN
1	A	207	ILE
1	A	209	LYS
1	A	211	GLN
1	A	225	ASP
1	A	241	LYS
1	A	244	ILE
1	A	248	THR
1	A	253	MET
1	A	259	PRO
1	A	263	LYS
1	A	270	LEU
1	A	276	SER
1	A	284	LEU
1	A	301	ASP
1	A	305	GLN
1	A	319	ASN
1	A	326	ASN
1	A	327	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	107	HIS
1	A	170	HIS
1	A	177	GLN
1	A	201	ASN
1	A	206	ASN
1	A	233	GLN
1	A	271	GLN

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Mol	Chain	Res	Type
1	A	305	GLN
1	A	319	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 carbohydrates 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, 95^{th} 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	331/331 (100%)	-1.03	1 (0%)	94	94	2, 6, 24, 46	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	GLY	3.5

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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.