



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 23, 2017 – 02:18 PM EST

PDB ID : 5TOT
Title : Crystal structure of AAT H143L:H189L double mutant
Authors : Mueser, T.C.; Dajnowicz, S.; Kovalevsky, A.
Deposited on : 2016-10-18
Resolution : 1.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

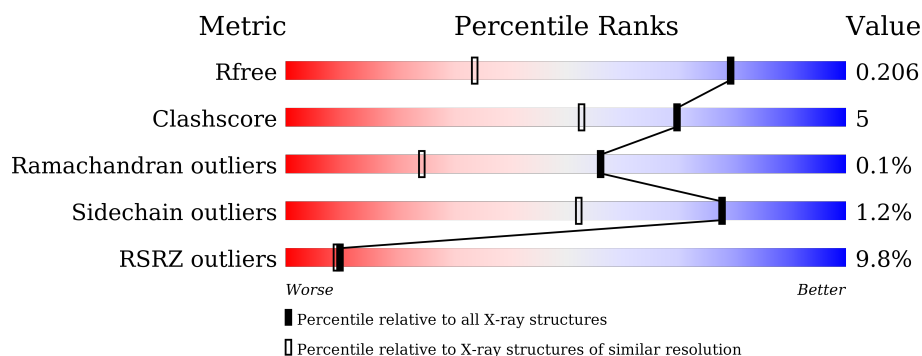
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	91344	1199 (1.40-1.40)
Clashscore	102246	1295 (1.40-1.40)
Ramachandran outliers	100387	1259 (1.40-1.40)
Sidechain outliers	100360	1258 (1.40-1.40)
RSRZ outliers	91569	1198 (1.40-1.40)

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. 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	414	<div> <div>3%</div> <div>93%</div> <div>7%</div> </div>
1	B	414	<div> <div>16%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7233 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 Aspartate aminotransferase, cytoplasmic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	P	S	0	3	0
			3316	2112	576	615	1	12			
1	B	397	Total	C	N	O	P	S	0	0	0
			3155	2009	551	582	1	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P00503
A	63	ASN	ASP	conflict	UNP P00503
A	143	LEU	HIS	engineered mutation	UNP P00503
A	189	LEU	HIS	engineered mutation	UNP P00503
A	288	GLN	GLU	conflict	UNP P00503
A	376	GLN	GLU	conflict	UNP P00503
B	-1	GLY	-	expression tag	UNP P00503
B	63	ASN	ASP	conflict	UNP P00503
B	143	LEU	HIS	engineered mutation	UNP P00503
B	189	LEU	HIS	engineered mutation	UNP P00503
B	288	GLN	GLU	conflict	UNP P00503
B	376	GLN	GLU	conflict	UNP P00503

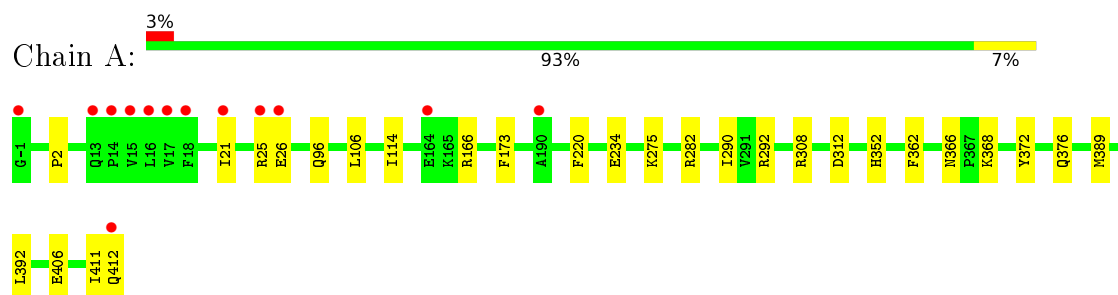
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	448	Total	O	0	0
			448	448		
2	B	314	Total	O	0	0
			314	314		

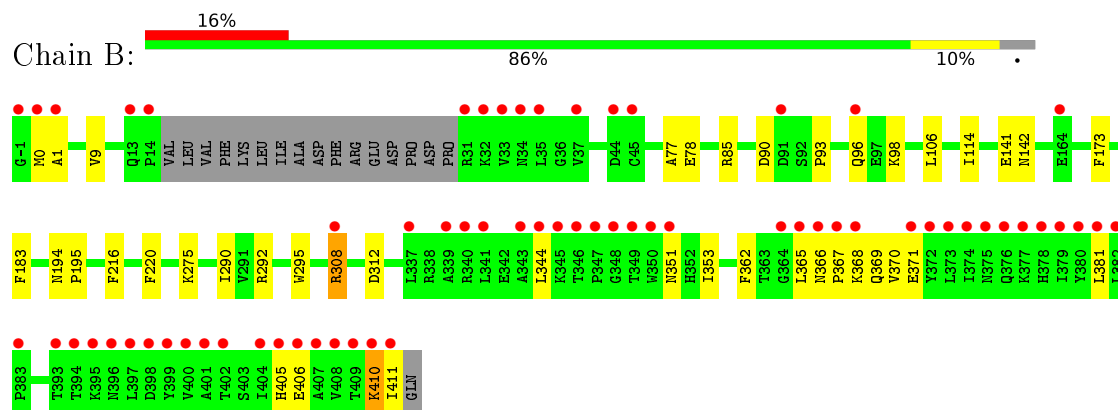
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Aspartate aminotransferase, cytoplasmic



- Molecule 1: Aspartate aminotransferase, cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.31Å 124.08Å 129.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.02 – 1.40 42.02 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (31.02-1.40) 99.8 (42.02-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 1.40Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.183 , 0.206 0.183 , 0.206	Depositor DCC
R_{free} test set	8734 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7233	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

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	0.34	0/3373	0.55	0/4582
1	B	0.38	1/3207 (0.0%)	0.56	1/4354 (0.0%)
All	All	0.36	1/6580 (0.0%)	0.56	1/8936 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	410	LYS	CD-CE	-5.07	1.38	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	ARG	NE-CZ-NH1	-8.20	116.20	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3316	0	3261	19	0
1	B	3155	0	3109	44	0
2	A	448	0	0	5	0
2	B	314	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7233	0	6370	58	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 5.

All (58) 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:366:ASN:ND2	1:A:412:GLN:OE1	2.02	0.91
1:B:85:ARG:NH1	1:B:90:ASP:OD1	2.06	0.88
1:B:410:LYS:NZ	1:B:411:ILE:HG13	1.89	0.86
1:B:78:GLU:OE1	2:B:502:HOH:O	1.94	0.85
1:B:141:GLU:OE2	2:B:501:HOH:O	1.94	0.84
1:A:308:ARG:HH21	1:A:312:ASP:HB2	1.54	0.71
1:B:371:GLU:OE2	1:B:371:GLU:N	2.25	0.68
1:B:410:LYS:HZ3	1:B:411:ILE:HG13	1.57	0.68
1:B:78:GLU:OE2	2:B:503:HOH:O	2.13	0.65
1:B:93:PRO:HA	1:B:96:GLN:HG2	1.80	0.63
1:B:308:ARG:HH12	1:B:312:ASP:HB2	1.64	0.63
1:B:353:ILE:N	2:B:504:HOH:O	2.19	0.63
1:A:234:GLU:OE2	2:A:501:HOH:O	2.15	0.62
1:A:21:ILE:O	1:A:25:ARG:HG3	1.98	0.62
1:A:411:ILE:O	1:A:412:GLN:HG2	1.99	0.62
1:A:389:MET:HE3	1:A:392:LEU:HD12	1.82	0.61
1:B:370:VAL:HG22	1:B:381:LEU:HD11	1.82	0.61
1:B:368:LYS:HA	1:B:371:GLU:OE2	2.01	0.60
1:B:353:ILE:HG12	2:B:504:HOH:O	2.00	0.60
1:A:292:ARG:NH1	2:A:504:HOH:O	2.36	0.58
1:B:308:ARG:NH1	2:B:510:HOH:O	2.37	0.57
1:B:410:LYS:HD3	1:B:411:ILE:N	2.20	0.55
2:A:504:HOH:O	1:B:142:ASN:ND2	2.40	0.54
1:B:308:ARG:HA	2:B:510:HOH:O	2.07	0.54
1:B:344:LEU:HB3	1:B:405:HIS:ND1	2.22	0.54
1:B:96:GLN:NE2	2:B:509:HOH:O	2.37	0.53
1:A:366:ASN:HD21	1:A:412:GLN:HB3	1.73	0.53
1:A:275:LYS:HZ1	1:B:1:ALA:HB3	1.74	0.52
1:B:410:LYS:HZ2	1:B:411:ILE:HG13	1.72	0.52
1:A:292:ARG:NH2	1:B:142:ASN:HB2	2.26	0.51
1:B:85:ARG:HG2	1:B:90:ASP:OD1	2.09	0.51
1:A:2:PRO:O	1:B:275:LYS:NZ	2.38	0.50
1:B:406:GLU:O	1:B:410:LYS:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:LYS:CE	1:B:411:ILE:HG13	2.42	0.49
1:A:106:LEU:HD11	1:B:106:LEU:HD11	1.95	0.48
1:B:93:PRO:HA	1:B:96:GLN:CG	2.43	0.48
1:B:367:PRO:O	1:B:371:GLU:OE2	2.32	0.48
1:B:410:LYS:HD3	1:B:410:LYS:C	2.34	0.48
1:A:372:TYR:CD1	1:A:376:GLN:HG3	2.49	0.47
1:A:96:GLN:HG2	2:A:508:HOH:O	2.13	0.46
1:B:77:ALA:HB3	2:B:502:HOH:O	2.15	0.46
1:B:98:LYS:HE2	1:B:98:LYS:HB3	1.54	0.45
1:A:368:LYS:HE3	1:A:368:LYS:HB2	1.80	0.44
1:B:292:ARG:NH2	2:B:515:HOH:O	2.50	0.44
1:A:282:ARG:HD2	1:B:9:VAL:O	2.18	0.44
1:A:114:ILE:HD12	1:A:290:ILE:HG22	2.00	0.43
1:B:106:LEU:HD23	1:B:295:TRP:CE2	2.54	0.43
1:B:114:ILE:HD12	1:B:290:ILE:HG22	2.00	0.43
1:B:366:ASN:HB2	1:B:367:PRO:HD2	2.00	0.43
1:A:406:GLU:HG3	2:A:651:HOH:O	2.19	0.43
1:B:183:PHE:HA	1:B:216:PHE:O	2.19	0.42
1:B:292:ARG:NH1	2:B:515:HOH:O	2.53	0.41
1:B:308:ARG:NH1	1:B:312:ASP:HB2	2.34	0.41
1:B:106:LEU:HD23	1:B:295:TRP:CD2	2.55	0.41
1:A:166:ARG:HD3	1:A:352:HIS:CE1	2.55	0.41
1:B:365:LEU:HG	1:B:369:GLN:HB2	2.03	0.41
1:B:410:LYS:HZ3	1:B:411:ILE:CG1	2.28	0.40
1:B:194:ASN:HA	1:B:195:PRO:HA	1.93	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	414/414 (100%)	406 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	392/414 (95%)	385 (98%)	6 (2%)	1 (0%)	46 19
All	All	806/828 (97%)	791 (98%)	14 (2%)	1 (0%)	56 24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	0	MET

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	355/352 (101%)	351 (99%)	4 (1%)	80 56
1	B	336/352 (96%)	332 (99%)	4 (1%)	78 52
All	All	691/704 (98%)	683 (99%)	8 (1%)	78 52

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	173	PHE
1	A	220	PHE
1	A	362	PHE
1	B	173	PHE
1	B	220	PHE
1	B	351	ASN
1	B	362	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	A	258	1	22,24,25	2.71	6 (27%)	28,32,34	1.23	3 (10%)
1	LLP	B	258	1	22,24,25	2.73	7 (31%)	28,32,34	1.28	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	258	1	-	0/15/17/19	0/1/1/1
1	LLP	B	258	1	-	0/15/17/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	258	LLP	C4-C5	-3.97	1.36	1.42
1	A	258	LLP	C4-C5	-3.38	1.37	1.42
1	B	258	LLP	C4-C3	-2.11	1.38	1.40
1	A	258	LLP	C6-N1	2.01	1.38	1.34
1	B	258	LLP	C5'-C5	2.02	1.56	1.51
1	A	258	LLP	C5'-C5	2.05	1.56	1.51
1	B	258	LLP	C6-N1	2.35	1.39	1.34
1	A	258	LLP	C2'-C2	2.64	1.55	1.50
1	B	258	LLP	C2'-C2	2.81	1.55	1.50
1	B	258	LLP	C4'-NZ	5.40	1.43	1.27
1	A	258	LLP	C4'-NZ	5.60	1.44	1.27
1	B	258	LLP	C4-C4'	8.95	1.61	1.46
1	A	258	LLP	C4-C4'	9.16	1.62	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	258	LLP	C4-C4'-NZ	-3.00	108.44	125.14
1	A	258	LLP	C4-C4'-NZ	-2.77	109.73	125.14
1	A	258	LLP	O-C-CA	-2.51	118.98	125.72
1	B	258	LLP	O-C-CA	-2.31	119.52	125.72
1	A	258	LLP	C5-C6-N1	-2.21	120.00	123.86
1	B	258	LLP	P-OP4-C5'	-2.21	115.68	120.79
1	B	258	LLP	C5-C6-N1	-2.20	120.02	123.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	413/414 (99%)	0.09	13 (3%)	52 49	7, 12, 28, 43	0
1	B	396/414 (95%)	0.89	66 (16%)	2 2	8, 17, 45, 61	5 (1%)
All	All	809/828 (97%)	0.48	79 (9%)	10 9	7, 14, 39, 61	5 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	GLY	18.1
1	B	0	MET	13.2
1	A	412	GLN	9.1
1	B	372	TYR	8.4
1	B	373	LEU	8.1
1	B	379	ILE	8.1
1	A	-1	GLY	7.0
1	B	409	THR	6.8
1	B	398	ASP	6.4
1	B	368	LYS	6.2
1	B	411	ILE	6.0
1	B	380	TYR	6.0
1	B	1	ALA	5.9
1	B	367	PRO	5.8
1	B	37	VAL	5.7
1	B	33	VAL	5.6
1	B	381	LEU	5.6
1	B	365	LEU	5.6
1	B	410	LYS	5.6
1	B	343	ALA	5.5
1	B	378	HIS	5.3
1	B	45	CYS	5.2
1	B	401	ALA	5.2
1	B	399	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	14	PRO	5.1
1	B	348	GLY	5.1
1	B	375	ASN	5.0
1	B	404	ILE	5.0
1	B	402	THR	5.0
1	B	31	ARG	4.8
1	B	400	VAL	4.7
1	B	397	LEU	4.7
1	B	366	ASN	4.6
1	B	344	LEU	4.6
1	B	374	ILE	4.6
1	B	364	GLY	4.6
1	B	349	THR	4.5
1	B	341	LEU	4.4
1	B	405	HIS	4.2
1	B	345	LYS	4.2
1	A	18	PHE	4.1
1	B	407	ALA	4.1
1	B	408	VAL	4.1
1	A	26	GLU	3.9
1	B	395	LYS	3.9
1	A	25	ARG	3.8
1	B	376	GLN	3.8
1	B	347	PRO	3.8
1	B	34	ASN	3.7
1	B	339	ALA	3.7
1	A	16	LEU	3.7
1	B	346	THR	3.6
1	B	350	TRP	3.5
1	B	371	GLU	3.5
1	B	13	GLN	3.5
1	B	32	LYS	3.4
1	A	15	VAL	3.3
1	B	382	LEU	3.3
1	B	377	LYS	3.2
1	B	44	ASP	3.0
1	B	406	GLU	3.0
1	B	383	PRO	3.0
1	B	394	THR	2.9
1	A	14	PRO	2.7
1	A	21	ILE	2.6
1	A	164	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	351	ASN	2.6
1	B	308	ARG	2.5
1	B	164	GLU	2.4
1	B	91	ASP	2.3
1	B	96	GLN	2.3
1	B	340	ARG	2.3
1	B	393	THR	2.3
1	B	35	LEU	2.3
1	A	17	VAL	2.3
1	B	337	LEU	2.2
1	A	13	GLN	2.1
1	B	396	ASN	2.1
1	A	190	ALA	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	LLP	B	258	24/25	0.97	0.09	-	8,11,16,20	0
1	LLP	A	258	24/25	0.98	0.10	-	6,9,12,18	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.