



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:22 pm BST

PDB ID : 1HKL
Title : FREE AND LIGANDED FORM OF AN ESTEROLYTIC CATALYTIC AN-TIBODY
Authors : Wedemayer, G.J.; Wang, L.H.; Patten, P.A.; Schultz, P.G.; Stevens, R.C.
Deposited on : 1996-12-20
Resolution : 2.68 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (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

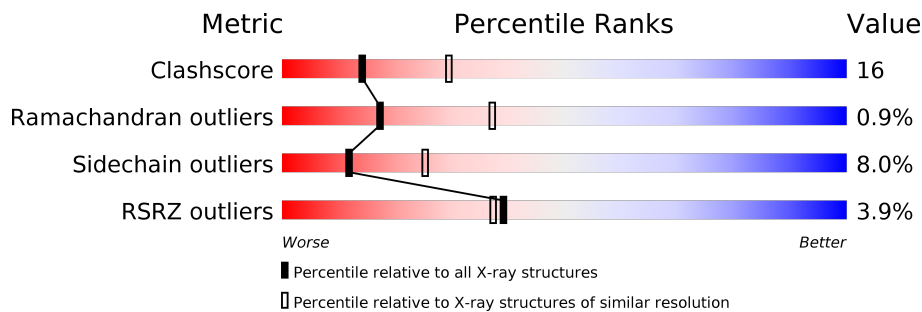
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 $\leq 5\%$. 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	L	214	 2% 64% 34%
2	H	217	 6% 63% 34%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4053 atoms, of which 771 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 48G7 FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	L	214	2045	1027	395	280	337	6	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	15	LEU	VAL	CONFLICT	UNP P01834
L	17	GLU	ASP	CONFLICT	UNP P01834
L	20	SER	THR	CONFLICT	UNP P01834
L	21	LEU	ILE	CONFLICT	UNP P01834
L	24	ARG	GLN	CONFLICT	UNP P01834
L	28	GLU	ASP	CONFLICT	UNP P01834
L	31	GLY	ASN	CONFLICT	UNP P01834
L	34	GLY	ASN	CONFLICT	UNP P01834
L	36	LEU	TYR	CONFLICT	UNP P01834
L	41	ASP	GLY	CONFLICT	UNP P01834
L	42	GLY	LYS	CONFLICT	UNP P01834
L	44	ILE	PRO	CONFLICT	UNP P01834
L	46	ARG	LEU	CONFLICT	UNP P01834
L	50	ALA	GLY	CONFLICT	UNP P01834
L	53	THR	ASN	CONFLICT	UNP P01834
L	55	HIS	GLU	CONFLICT	UNP P01834
L	56	SER	THR	CONFLICT	UNP P01834
L	60	LYS	SER	CONFLICT	UNP P01834
L	66	ARG	GLY	CONFLICT	UNP P01834
L	69	SER	THR	CONFLICT	UNP P01834
L	71	TYR	PHE	CONFLICT	UNP P01834
L	72	SER	ILE	CONFLICT	UNP P01834
L	73	LEU	PHE	CONFLICT	UNP P01834
L	79	GLU	GLN	CONFLICT	UNP P01834
L	80	SER	PRO	CONFLICT	UNP P01834
L	83	PHE	ILE	CONFLICT	UNP P01834
L	85	ASP	THR	CONFLICT	UNP P01834

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Chain	Residue	Modelled	Actual	Comment	Reference
L	89	LEU	GLN	CONFLICT	UNP P01834
L	92	ALA	ASP	CONFLICT	UNP P01834
L	93	SER	ASN	CONFLICT	UNP P01834
L	94	TYR	LEU	CONFLICT	UNP P01834
L	96	ARG	LEU	CONFLICT	UNP P01834
L	177	SER	ASN	CONFLICT	UNP P01834

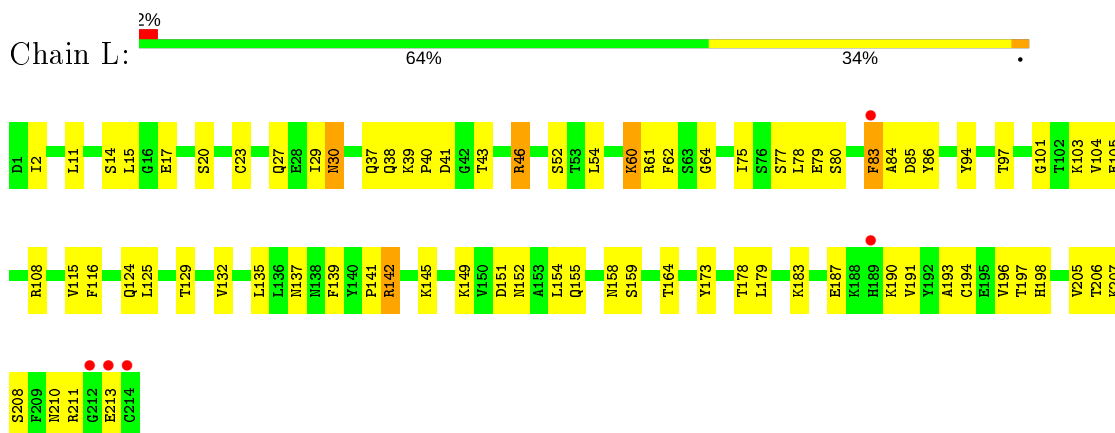
- Molecule 2 is a protein called 48G7 FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	H	217	2008	1031	376	267	328	6	0	0	0

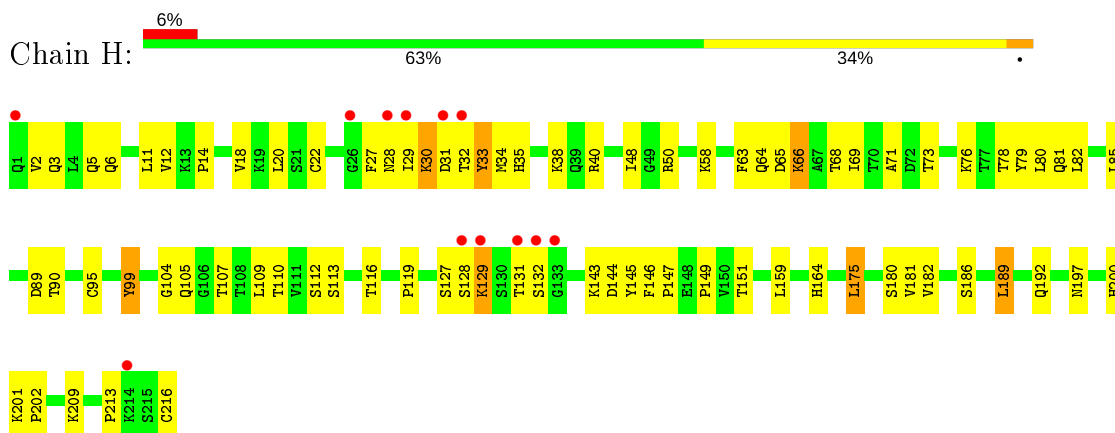
3 Residue-property plots [i](#)

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: 48G7 FAB



- Molecule 2: 48G7 FAB



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.69Å 44.49Å 84.95Å 90.00° 121.75° 90.00°	Depositor
Resolution (Å)	6.00 – 2.68 19.68 – 2.68	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.68) 80.4 (19.68-2.68)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.67Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , 0.244 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtrriage
Anisotropy	0.588	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4053	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.12% 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](#)

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	L	0.35	0/1683	0.64	0/2277
2	H	0.35	0/1671	0.65	0/2278
All	All	0.35	0/3354	0.64	0/4555

There are no bond length outliers.

There are no bond angle outliers.

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	L	1650	395	1601	50	0
2	H	1632	376	1611	55	0
All	All	3282	771	3212	101	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 16.

All (101) 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:H:29:ILE:HD11	2:H:73:THR:HA	1.43	0.96
1:L:39:LYS:HE2	1:L:40:PRO:HD2	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:PRO:O	1:L:198:HIS:HE1	1.75	0.69
1:L:2:ILE:HG12	1:L:27:GLN:HB2	1.75	0.68
1:L:145:LYS:HB3	1:L:197:THR:HB	1.77	0.67
1:L:196:VAL:HG22	1:L:205:VAL:HG22	1.75	0.67
2:H:90:THR:HG23	2:H:110:THR:HA	1.78	0.66
1:L:187:GLU:HA	1:L:211:ARG:HD2	1.79	0.65
2:H:71:ALA:HB2	2:H:78:THR:HG22	1.79	0.65
2:H:6:GLN:HE21	2:H:104:GLY:HA3	1.62	0.64
1:L:115:VAL:HG21	1:L:196:VAL:HG21	1.80	0.62
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.81	0.62
1:L:11:LEU:HD22	1:L:104:VAL:HG12	1.82	0.61
1:L:125:LEU:O	1:L:183:LYS:HD2	2.03	0.59
1:L:61:ARG:HD2	1:L:77:SER:O	2.02	0.59
1:L:37:GLN:HA	1:L:85:ASP:O	2.02	0.58
1:L:135:LEU:HD11	1:L:137:ASN:HB2	1.86	0.57
1:L:159:SER:HA	1:L:178:THR:O	2.06	0.56
1:L:151:ASP:HA	1:L:191:VAL:HG23	1.86	0.56
1:L:124:GLN:HG2	1:L:129:THR:O	2.06	0.56
2:H:127:SER:OG	2:H:213:PRO:HB3	2.06	0.55
1:L:85:ASP:OD1	1:L:103:LYS:HD2	2.06	0.55
1:L:2:ILE:HG23	1:L:27:GLN:H	1.73	0.54
2:H:129:LYS:HA	2:H:129:LYS:HE2	1.89	0.54
2:H:18:VAL:HG13	2:H:85:LEU:HD11	1.90	0.54
1:L:149:LYS:HE2	1:L:154:LEU:HG	1.89	0.54
2:H:5:GLN:O	2:H:22:CYS:HA	2.07	0.54
1:L:54:LEU:HD21	1:L:62:PHE:O	2.07	0.54
1:L:194:CYS:O	1:L:206:THR:HA	2.09	0.53
1:L:191:VAL:HG12	1:L:210:ASN:ND2	2.23	0.53
1:L:196:VAL:CG2	1:L:205:VAL:HG22	2.40	0.51
2:H:147:PRO:O	2:H:200:HIS:HE1	1.93	0.51
1:L:2:ILE:HD13	1:L:29:ILE:HG22	1.92	0.51
1:L:40:PRO:O	1:L:41:ASP:HB2	2.10	0.51
1:L:61:ARG:O	1:L:75:ILE:HA	2.12	0.50
2:H:18:VAL:HG13	2:H:85:LEU:CD1	2.43	0.49
2:H:201:LYS:HB2	2:H:202:PRO:HD3	1.95	0.49
1:L:38:GLN:HA	1:L:43:THR:O	2.13	0.49
1:L:135:LEU:HG	2:H:181:VAL:HG11	1.96	0.48
2:H:12:VAL:HG11	2:H:18:VAL:HG12	1.94	0.48
1:L:151:ASP:O	1:L:152:ASN:HB2	2.13	0.48
2:H:132:SER:HA	2:H:186:SER:HB3	1.96	0.48
1:L:15:LEU:HD11	1:L:80:SER:OG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:MET:HB2	2:H:78:THR:HG21	1.96	0.48
2:H:2:VAL:HB	2:H:27:PHE:CE2	2.49	0.47
2:H:105:GLN:OE1	2:H:105:GLN:N	2.47	0.47
2:H:66:LYS:N	2:H:66:LYS:HD3	2.30	0.47
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.97	0.47
1:L:94:TYR:CD1	2:H:58:LYS:HG2	2.49	0.47
1:L:116:PHE:HD2	1:L:135:LEU:HD12	1.80	0.47
1:L:151:ASP:HA	1:L:191:VAL:CG2	2.44	0.47
2:H:2:VAL:HB	2:H:27:PHE:CD2	2.50	0.47
2:H:28:ASN:HB2	2:H:76:LYS:HG2	1.97	0.46
2:H:33:TYR:HD1	2:H:33:TYR:O	1.98	0.46
2:H:128:SER:HA	2:H:216:CYS:O	2.16	0.46
2:H:14:PRO:HD3	2:H:112:SER:O	2.16	0.46
2:H:33:TYR:HD1	2:H:33:TYR:C	2.19	0.46
2:H:164:HIS:O	2:H:180:SER:HA	2.15	0.46
1:L:17:GLU:O	1:L:78:LEU:HB2	2.16	0.46
2:H:68:THR:HB	2:H:81:GLN:HB3	1.97	0.46
1:L:52:SER:HB3	1:L:64:GLY:O	2.16	0.45
2:H:35:HIS:O	2:H:95:CYS:HA	2.17	0.45
2:H:147:PRO:O	2:H:200:HIS:CE1	2.68	0.45
2:H:33:TYR:CD1	2:H:33:TYR:C	2.90	0.45
1:L:193:ALA:HB2	1:L:208:SER:HB3	1.99	0.45
2:H:132:SER:C	2:H:186:SER:HB3	2.38	0.44
2:H:18:VAL:HG22	2:H:82:LEU:HB2	1.99	0.44
2:H:27:PHE:HB2	2:H:32:THR:HG1	1.82	0.44
1:L:125:LEU:HB3	1:L:183:LYS:NZ	2.33	0.44
2:H:28:ASN:OD1	2:H:30:LYS:HB2	2.18	0.44
2:H:69:ILE:HA	2:H:79:TYR:O	2.18	0.43
1:L:46:ARG:HH21	2:H:99:TYR:HD2	1.64	0.43
1:L:132:VAL:HB	1:L:179:LEU:HB3	2.00	0.43
2:H:28:ASN:CB	2:H:76:LYS:HG2	2.49	0.43
2:H:12:VAL:HG21	2:H:85:LEU:HD13	2.00	0.43
1:L:94:TYR:CG	2:H:58:LYS:HG2	2.54	0.43
2:H:85:LEU:HA	2:H:89:ASP:OD2	2.19	0.42
2:H:11:LEU:HD21	2:H:146:PHE:HE1	1.84	0.42
2:H:6:GLN:HE21	2:H:104:GLY:CA	2.30	0.42
2:H:20:LEU:HD12	2:H:80:LEU:HD23	2.01	0.42
1:L:115:VAL:HA	1:L:135:LEU:O	2.20	0.42
2:H:144:ASP:HA	2:H:175:LEU:HB3	2.01	0.42
1:L:139:PHE:HD2	1:L:198:HIS:CE1	2.38	0.42
1:L:14:SER:O	1:L:17:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:ARG:HB3	1:L:173:TYR:CE2	2.55	0.42
2:H:119:PRO:HB3	2:H:145:TYR:HB3	2.01	0.41
2:H:131:THR:HG23	2:H:131:THR:O	2.20	0.41
2:H:64:GLN:O	2:H:65:ASP:HB2	2.20	0.41
1:L:155:GLN:HB3	1:L:158:ASN:HD21	1.85	0.41
1:L:39:LYS:HD2	1:L:84:ALA:HB2	2.02	0.41
1:L:207:LYS:HD3	1:L:207:LYS:HA	1.82	0.41
2:H:116:THR:HA	2:H:146:PHE:O	2.20	0.41
2:H:143:LYS:HE3	2:H:143:LYS:HB2	1.78	0.41
2:H:189:LEU:HB3	2:H:213:PRO:HG2	2.03	0.41
1:L:83:PHE:CD1	1:L:104:VAL:O	2.74	0.41
2:H:48:ILE:HA	2:H:63:PHE:CD2	2.56	0.41
2:H:6:GLN:HB2	2:H:105:GLN:NE2	2.36	0.41
1:L:86:TYR:O	1:L:101:GLY:HA2	2.21	0.40
2:H:129:LYS:HG3	2:H:129:LYS:O	2.21	0.40
1:L:141:PRO:O	1:L:198:HIS:CE1	2.64	0.40
1:L:60:LYS:N	1:L:60:LYS:HD2	2.35	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	L	212/214 (99%)	190 (90%)	20 (9%)	2 (1%)	17	37
2	H	215/217 (99%)	194 (90%)	19 (9%)	2 (1%)	17	37
All	All	427/431 (99%)	384 (90%)	39 (9%)	4 (1%)	17	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	30	ASN

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Mol	Chain	Res	Type
2	H	149	PRO
2	H	189	LEU
1	L	213	GLU

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	L	187/187 (100%)	174 (93%)	13 (7%)	15	32
2	H	187/187 (100%)	170 (91%)	17 (9%)	9	20
All	All	374/374 (100%)	344 (92%)	30 (8%)	12	25

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	SER
1	L	23	CYS
1	L	30	ASN
1	L	46	ARG
1	L	60	LYS
1	L	79	GLU
1	L	83	PHE
1	L	97	THR
1	L	105	GLU
1	L	108	ARG
1	L	142	ARG
1	L	164	THR
1	L	190	LYS
2	H	3	GLN
2	H	30	LYS
2	H	31	ASP
2	H	33	TYR
2	H	40	ARG
2	H	50	ARG
2	H	66	LYS

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Mol	Chain	Res	Type
2	H	99	TYR
2	H	107	THR
2	H	109	LEU
2	H	113	SER
2	H	129	LYS
2	H	151	THR
2	H	175	LEU
2	H	192	GLN
2	H	197	ASN
2	H	209	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	30	ASN
1	L	37	GLN
1	L	198	HIS
1	L	210	ASN
2	H	6	GLN
2	H	200	HIS
2	H	204	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 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 [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	L	214/214 (100%)	-0.06	5 (2%) 60 60	3, 13, 29, 57	0
2	H	217/217 (100%)	0.09	12 (5%) 25 23	2, 13, 48, 64	0
All	All	431/431 (100%)	0.02	17 (3%) 39 37	2, 13, 40, 64	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	214	CYS	9.9
2	H	132	SER	7.4
2	H	131	THR	5.8
2	H	128	SER	4.6
2	H	32	THR	3.9
2	H	129	LYS	3.5
2	H	28	ASN	3.3
1	L	213	GLU	3.3
1	L	212	GLY	3.2
2	H	1	GLN	2.8
2	H	214	LYS	2.8
2	H	26	GLY	2.6
2	H	133	GLY	2.5
2	H	29	ILE	2.4
2	H	31	ASP	2.3
1	L	83	PHE	2.2
1	L	189	HIS	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 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.