



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:35 AM UTC

PDB ID : 4B6H / pdb_00004b6h
Title : Structure of hDcp1a in complex with proline rich sequence of PNRC2
Authors : Lai, T.; Song, H.
Deposited on : 2012-08-13
Resolution : 2.60 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

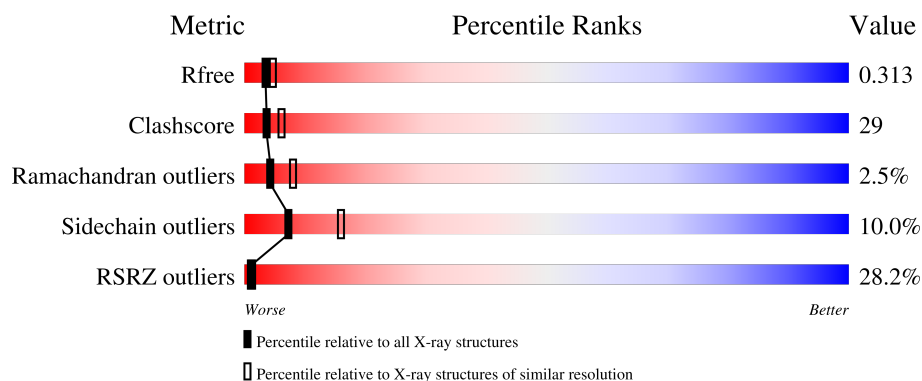
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	134	9% 51% 39% 5%
1	B	134	32% 40% 27% 8% 25%
2	C	135	4% 5% 89%
2	D	135	9% 5% 90%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2152 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 MRNA-DECAPPING ENZYME 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1052	673	177	196	6			
1	B	101	Total	C	N	O	S	0	0	1
			823	535	134	150	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	expression tag	UNP Q9NPI6
A	-2	ALA	-	expression tag	UNP Q9NPI6
A	-1	ASP	-	expression tag	UNP Q9NPI6
A	0	LEU	-	expression tag	UNP Q9NPI6
B	-3	MET	-	expression tag	UNP Q9NPI6
B	-2	ALA	-	expression tag	UNP Q9NPI6
B	-1	ASP	-	expression tag	UNP Q9NPI6
B	0	LEU	-	expression tag	UNP Q9NPI6

- Molecule 2 is a protein called PROLINE-RICH NUCLEAR RECEPTOR COACTIVATOR 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	0	0	1
			109	73	19	17			
2	D	14	Total	C	N	O	0	0	1
			102	68	18	16			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	MET	-	expression tag	UNP Q9NPJ4
C	-12	GLY	-	expression tag	UNP Q9NPJ4
C	-11	SER	-	expression tag	UNP Q9NPJ4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	SER	-	expression tag	UNP Q9NPJ4
C	-9	HIS	-	expression tag	UNP Q9NPJ4
C	-8	HIS	-	expression tag	UNP Q9NPJ4
C	-7	HIS	-	expression tag	UNP Q9NPJ4
C	-6	HIS	-	expression tag	UNP Q9NPJ4
C	-5	HIS	-	expression tag	UNP Q9NPJ4
C	-4	HIS	-	expression tag	UNP Q9NPJ4
C	-3	SER	-	expression tag	UNP Q9NPJ4
C	-2	GLN	-	expression tag	UNP Q9NPJ4
C	-1	ASP	-	expression tag	UNP Q9NPJ4
C	0	PRO	-	expression tag	UNP Q9NPJ4
D	-13	MET	-	expression tag	UNP Q9NPJ4
D	-12	GLY	-	expression tag	UNP Q9NPJ4
D	-11	SER	-	expression tag	UNP Q9NPJ4
D	-10	SER	-	expression tag	UNP Q9NPJ4
D	-9	HIS	-	expression tag	UNP Q9NPJ4
D	-8	HIS	-	expression tag	UNP Q9NPJ4
D	-7	HIS	-	expression tag	UNP Q9NPJ4
D	-6	HIS	-	expression tag	UNP Q9NPJ4
D	-5	HIS	-	expression tag	UNP Q9NPJ4
D	-4	HIS	-	expression tag	UNP Q9NPJ4
D	-3	SER	-	expression tag	UNP Q9NPJ4
D	-2	GLN	-	expression tag	UNP Q9NPJ4
D	-1	ASP	-	expression tag	UNP Q9NPJ4
D	0	PRO	-	expression tag	UNP Q9NPJ4

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	34	Total O 34 34	0	0
3	B	25	Total O 25 25	0	0
3	C	4	Total O 4 4	0	0
3	D	3	Total O 3 3	0	0

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	76.09Å 97.64Å 109.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.93 – 2.60 72.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (72.93-2.60) 97.6 (72.93-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.62Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.1_357)	Depositor
R, R_{free}	0.234 , 0.285 0.277 , 0.313	Depositor DCC
R_{free} test set	1262 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 103.9	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	0.90	EDS
Total number of atoms	2152	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% 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	A	0.51	0/1077	0.95	3/1459 (0.2%)
1	B	0.56	1/842 (0.1%)	0.92	3/1140 (0.3%)
2	C	0.83	1/116 (0.9%)	1.22	2/162 (1.2%)
2	D	0.79	1/107 (0.9%)	0.67	0/147
All	All	0.57	3/2142 (0.1%)	0.94	8/2908 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	115	VAL	C-N	-6.86	1.23	1.34
2	C	115	VAL	C-N	-6.66	1.23	1.34
1	B	126	VAL	C-N	-6.57	1.24	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	PRO	CA-N-CD	-9.28	99.01	112.00
1	A	20	ASP	CA-C-N	8.91	129.13	119.87
1	A	20	ASP	C-N-CA	8.91	129.13	119.87
2	C	103	SER	CA-C-N	-7.80	111.74	119.78
2	C	103	SER	C-N-CA	-7.80	111.74	119.78
1	B	22	TYR	CA-C-N	5.71	131.98	121.70
1	B	22	TYR	C-N-CA	5.71	131.98	121.70
1	A	75	MET	N-CA-C	5.43	119.54	113.02

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	1052	0	1023	59	2
1	B	823	0	794	49	1
2	C	109	0	109	10	0
2	D	102	0	101	11	0
3	A	34	0	0	10	3
3	B	25	0	0	16	0
3	C	4	0	0	0	0
3	D	3	0	0	2	0
All	All	2152	0	2027	120	3

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 29.

All (120) 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:75:MET:HE2	1:A:75:MET:O	1.12	1.27
1:B:71:ASN:HB3	1:B:74:ASN:O	1.35	1.25
1:A:75:MET:O	1:A:75:MET:CE	2.03	1.07
1:A:72:ARG:NH2	3:A:2017:HOH:O	1.87	1.05
1:A:57:TYR:HE2	1:A:68:THR:HG22	1.20	1.02
2:D:106:VAL:O	2:D:106:VAL:HG13	1.68	0.92
1:B:44:GLN:HE21	1:B:44:GLN:N	1.69	0.88
2:D:115:VAL:O	3:D:2002:HOH:O	1.91	0.88
1:B:49:ASP:HA	3:B:2010:HOH:O	1.74	0.87
2:D:116:PRO:N	3:D:2003:HOH:O	2.07	0.87
1:A:44:GLN:HE21	1:A:44:GLN:H	1.20	0.86
1:B:82:VAL:HG11	1:B:125:VAL:HG23	1.55	0.86
1:B:23:ILE:N	3:B:2004:HOH:O	2.08	0.85
1:A:44:GLN:HE21	1:A:44:GLN:N	1.74	0.85
1:A:91:HIS:ND1	3:A:2029:HOH:O	2.08	0.85
1:A:75:MET:HE2	1:A:75:MET:C	2.02	0.84
1:A:42:ALA:CB	1:A:44:GLN:HE22	1.89	0.84
1:A:42:ALA:HB3	1:A:44:GLN:HE22	1.43	0.84
1:A:57:TYR:CE2	1:A:68:THR:HG22	2.11	0.82
1:A:91:HIS:CG	3:A:2029:HOH:O	2.30	0.82
2:C:106:VAL:HG13	2:C:106:VAL:O	1.81	0.79
1:B:82:VAL:O	1:B:82:VAL:HG12	1.84	0.78
1:B:44:GLN:CA	3:B:2009:HOH:O	2.31	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLN:N	3:B:2009:HOH:O	2.19	0.76
2:C:104:PRO:O	2:C:106:VAL:N	2.18	0.76
1:A:92:GLU:OE1	3:A:2030:HOH:O	2.04	0.75
1:B:71:ASN:CB	1:B:74:ASN:O	2.28	0.72
1:B:71:ASN:ND2	3:B:2013:HOH:O	1.99	0.71
1:B:80:GLU:OE1	3:B:2014:HOH:O	2.10	0.69
1:A:128:GLU:OE1	1:A:128:GLU:HA	1.93	0.69
1:B:62:SER:HB2	1:B:64:TYR:CE1	2.26	0.69
1:B:49:ASP:CA	3:B:2010:HOH:O	2.35	0.69
1:B:89:GLN:OE1	3:B:2017:HOH:O	2.10	0.68
1:B:94:PHE:CE1	2:D:107:LEU:HD22	2.29	0.68
1:A:82:VAL:HG11	1:A:125:VAL:HG23	1.76	0.67
2:D:106:VAL:O	2:D:106:VAL:CG1	2.41	0.67
1:B:101:SER:HG	1:B:103:SER:HG	1.37	0.66
1:A:62:SER:HB2	1:A:64:TYR:CE1	2.30	0.66
1:B:71:ASN:HB2	3:B:2013:HOH:O	1.95	0.66
1:B:87:GLU:CD	1:B:98:ARG:HH21	2.03	0.65
1:B:94:PHE:CZ	2:D:107:LEU:HD22	2.30	0.65
2:D:107:LEU:HD23	2:D:107:LEU:N	2.13	0.64
1:B:22:TYR:HA	1:B:23:ILE:HB	1.80	0.63
1:A:49:ASP:HA	3:A:2015:HOH:O	2.00	0.62
1:B:44:GLN:N	1:B:44:GLN:NE2	2.44	0.61
1:B:114:ASP:O	1:B:118:ILE:HG12	2.01	0.60
1:A:92:GLU:HB3	1:A:112:LYS:NZ	2.16	0.60
1:A:82:VAL:O	1:A:129:GLU:HG3	2.03	0.59
1:A:65:HIS:HD2	3:A:2035:HOH:O	1.85	0.59
1:B:44:GLN:HA	3:B:2009:HOH:O	1.98	0.58
1:A:128:GLU:HG3	3:A:2033:HOH:O	2.03	0.58
1:A:67:PHE:CD1	1:A:122:MET:HE1	2.38	0.58
1:B:60:SER:O	1:B:61:ALA:HB2	2.03	0.57
1:A:36:TYR:CG	2:C:107:LEU:HD11	2.39	0.57
1:A:44:GLN:N	1:A:44:GLN:NE2	2.48	0.56
1:B:21:PRO:HD2	1:B:21:PRO:O	2.04	0.56
1:A:60:SER:O	1:A:61:ALA:HB2	2.04	0.56
1:B:87:GLU:HG3	2:D:114:TRP:CZ2	2.41	0.56
1:A:90:LEU:HD11	1:A:92:GLU:HG3	1.86	0.56
1:A:101:SER:O	1:A:102:LEU:HB2	2.06	0.55
1:B:71:ASN:CB	3:B:2013:HOH:O	2.52	0.55
2:C:106:VAL:O	2:C:106:VAL:CG1	2.54	0.55
1:A:87:GLU:CD	1:A:98:ARG:HH21	2.15	0.54
1:A:94:PHE:CE1	2:C:107:LEU:HD22	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:THR:HB	3:B:2006:HOH:O	2.08	0.53
1:B:127:GLU:N	3:B:2023:HOH:O	2.42	0.53
1:A:45:TRP:NE1	2:C:108:PRO:O	2.39	0.52
1:B:91:HIS:HB3	2:D:108:PRO:HG3	1.91	0.52
1:A:37:THR:HG22	1:A:105:TYR:CE1	2.45	0.51
1:A:2:GLU:HA	1:A:5:SER:HB3	1.92	0.51
1:B:38:PHE:HB3	1:B:104:ILE:HB	1.92	0.50
3:A:2027:HOH:O	2:C:109:LYS:O	2.20	0.50
2:C:107:LEU:HB3	2:C:108:PRO:HD2	1.92	0.50
1:A:33:VAL:HG21	1:A:54:LEU:HB2	1.94	0.49
1:A:37:THR:HG22	1:A:105:TYR:CD1	2.47	0.49
1:B:101:SER:O	1:B:102:LEU:HB2	2.13	0.49
1:A:16:LEU:CD2	1:A:68:THR:HG21	2.44	0.48
1:A:44:GLN:H	1:A:44:GLN:NE2	2.01	0.48
1:B:69:ILE:HB	1:B:78:LEU:HB3	1.96	0.48
1:B:126:VAL:HG12	1:B:127:GLU:N	2.27	0.48
1:B:37:THR:HG23	1:B:48:THR:CG2	2.43	0.48
2:D:102:PRO:O	2:D:103:SER:C	2.57	0.48
1:A:118:ILE:O	1:A:122:MET:HG2	2.14	0.47
1:B:47:LYS:NZ	3:B:2010:HOH:O	2.48	0.47
1:B:71:ASN:CG	1:B:74:ASN:N	2.72	0.47
1:B:33:VAL:HG21	1:B:54:LEU:HB2	1.97	0.47
1:A:71:ASN:ND2	1:A:74:ASN:OD1	2.49	0.47
1:B:48:THR:C	3:B:2010:HOH:O	2.59	0.46
1:A:20:ASP:OD1	1:A:20:ASP:C	2.58	0.46
1:A:16:LEU:HD22	1:A:68:THR:HG21	1.98	0.45
3:A:2024:HOH:O	2:C:113:HIS:HE1	1.98	0.45
1:A:17:LYS:HD3	1:A:23:ILE:O	2.17	0.45
1:B:42:ALA:HB3	1:B:44:GLN:HE22	1.82	0.45
1:A:38:PHE:O	3:A:2012:HOH:O	2.21	0.44
1:B:67:PHE:CD1	1:B:122:MET:HE1	2.52	0.44
1:A:52:GLY:HA2	1:A:72:ARG:HG2	2.00	0.44
1:A:75:MET:HE3	1:A:75:MET:HB2	1.57	0.44
1:A:42:ALA:HB1	1:A:44:GLN:HE22	1.80	0.44
1:A:38:PHE:HB3	1:A:104:ILE:HB	1.99	0.43
1:A:112:LYS:HE3	1:A:112:LYS:HB2	1.45	0.43
1:A:87:GLU:HG3	2:C:114:TRP:CZ2	2.53	0.43
1:A:114:ASP:O	1:A:118:ILE:HG12	2.19	0.43
2:D:107:LEU:HB3	2:D:108:PRO:HD2	2.00	0.42
1:B:82:VAL:HG11	1:B:125:VAL:CG2	2.38	0.42
1:A:20:ASP:HA	1:A:21:PRO:HD3	1.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PHE:CG	1:A:122:MET:HE1	2.55	0.42
1:A:59:ARG:HD3	1:A:63:PRO:O	2.20	0.42
1:B:60:SER:O	1:B:61:ALA:CB	2.68	0.42
1:B:37:THR:HG23	1:B:48:THR:HG22	2.01	0.41
1:A:20:ASP:O	1:A:23:ILE:HG13	2.20	0.41
1:B:83:ASN:HB2	1:B:84:LYS:HE2	2.01	0.41
1:A:68:THR:HA	1:A:78:LEU:O	2.21	0.41
1:A:80:GLU:HA	1:A:81:PRO:HD3	1.92	0.41
1:B:71:ASN:OD1	1:B:74:ASN:N	2.53	0.41
1:A:30:THR:O	1:A:53:THR:HG23	2.20	0.41
1:B:109:PHE:HB2	1:B:115:CYS:HB2	2.03	0.41
1:A:65:HIS:HB2	1:A:82:VAL:HB	2.03	0.41
1:A:21:PRO:HG3	1:B:83:ASN:ND2	2.36	0.40
1:B:113:ASN:ND2	3:B:2021:HOH:O	2.41	0.40
1:A:6:ARG:O	1:A:10:GLU:HG3	2.21	0.40

All (3) 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)
1:A:1:MET:CG	3:A:2017:HOH:O[3_555]	2.00	0.20
1:B:92:GLU:OE2	3:A:2032:HOH:O[7_445]	2.00	0.20
1:A:1:MET:CB	3:A:2017:HOH:O[3_555]	2.04	0.16

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	125/134 (93%)	115 (92%)	8 (6%)	2 (2%)	7	16
1	B	92/134 (69%)	84 (91%)	5 (5%)	3 (3%)	3	5
2	C	13/135 (10%)	9 (69%)	3 (23%)	1 (8%)	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	10/135 (7%)	9 (90%)	1 (10%)	0	100	100
All	All	240/538 (45%)	217 (90%)	17 (7%)	6 (2%)	4	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	105	SER
1	B	31	GLY
1	A	61	ALA
1	B	61	ALA
1	B	23	ILE
1	A	31	GLY

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	114/118 (97%)	106 (93%)	8 (7%)	14	31
1	B	90/118 (76%)	80 (89%)	10 (11%)	6	12
2	C	14/117 (12%)	11 (79%)	3 (21%)	1	2
2	D	13/117 (11%)	11 (85%)	2 (15%)	2	5
All	All	231/470 (49%)	208 (90%)	23 (10%)	7	16

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	18	GLN
1	A	44	GLN
1	A	68	THR
1	A	75	MET
1	A	84	LYS
1	A	98	ARG
1	A	128	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	30	THR
1	B	44	GLN
1	B	68	THR
1	B	75	MET
1	B	84	LYS
1	B	89	GLN
1	B	98	ARG
1	B	103	SER
1	B	122	MET
1	B	126	VAL
2	C	103	SER
2	C	105	SER
2	C	107	LEU
2	D	105	SER
2	D	107	LEU

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

Mol	Chain	Res	Type
1	A	44	GLN
1	A	65	HIS
1	A	89	GLN
1	B	32	GLN
1	B	74	ASN
1	B	89	GLN
2	D	113	HIS

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 oligosaccharides 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, 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	129/134 (96%)	0.84	12 (9%) 14 11	49, 73, 107, 138	0
1	B	101/134 (75%)	2.05	43 (42%) 0 0	56, 87, 127, 168	0
2	C	15/135 (11%)	1.60	6 (40%) 1 0	65, 80, 114, 124	0
2	D	14/135 (10%)	2.91	12 (85%) 0 0	82, 115, 132, 146	0
All	All	259/538 (48%)	1.47	73 (28%) 1 1	49, 81, 124, 168	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	TYR	8.4
1	B	21	PRO	7.1
1	B	61	ALA	6.5
1	B	60	SER	5.1
2	D	116	PRO	4.8
1	B	45	TRP	4.1
2	D	111	PRO	4.1
1	B	42	ALA	4.1
1	B	98	ARG	3.6
1	B	74	ASN	3.5
1	B	125	VAL	3.5
1	B	64	TYR	3.4
1	B	105	TYR	3.4
2	C	104	PRO	3.3
1	B	103	SER	3.3
1	B	46	GLU	3.3
2	D	112	SER	3.2
2	C	106	VAL	3.2
1	B	31	GLY	3.2
1	B	101	SER	3.2
2	D	105	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	50	ILE	3.1
2	D	113	HIS	3.0
1	A	47	LYS	3.0
1	B	36	TYR	3.0
1	A	49	ASP	3.0
2	D	109	LYS	3.0
1	B	104	ILE	3.0
1	B	102	LEU	3.0
1	B	71	ASN	3.0
1	B	58	ARG	2.9
1	A	59	ARG	2.8
2	D	114	TRP	2.8
1	B	93	PRO	2.8
1	B	107	ILE	2.8
1	B	124	ASP	2.8
1	B	92	GLU	2.8
2	D	103	SER	2.7
1	B	110	TYR	2.7
1	B	75	MET	2.7
2	D	115	VAL	2.7
1	A	62	SER	2.6
2	D	106	VAL	2.6
1	A	84	LYS	2.6
1	B	39	CYS	2.6
1	B	38	PHE	2.6
1	B	123	ALA	2.6
2	D	110	PRO	2.5
2	D	107	LEU	2.5
1	B	97	TYR	2.5
1	B	32	GLN	2.5
1	B	77	ASN	2.4
1	B	99	ASN	2.4
1	B	59	ARG	2.4
1	A	71	ASN	2.4
1	B	70	VAL	2.4
2	C	116	PRO	2.3
1	B	55	PHE	2.3
1	A	113	ASN	2.3
1	A	64	TYR	2.3
2	C	115	VAL	2.3
1	B	62	SER	2.2
1	A	19	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	94	PHE	2.2
2	C	105	SER	2.2
1	B	119	ALA	2.1
1	B	37	THR	2.1
1	A	63	PRO	2.1
2	C	102	PRO	2.1
1	B	69	ILE	2.0
1	A	100	ALA	2.0
1	A	60	SER	2.0
1	B	108	TRP	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 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.