



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 05:16 PM GMT

PDB ID : 2C9T
Title : CRYSTAL STRUCTURE OF ACETYLCHOLINE BINDING PROTEIN (ACHBP) FROM APLYSIA CALIFORNICA IN COMPLEX WITH ALPHA-CONOTOXIN IMI
Authors : Ulens, C.; Hogg, R.C.; Celie, P.H.; Bertrand, D.; Tsetlin, V.; Smit, A.B.; Sixma, T.K.
Deposited on : 2005-12-14
Resolution : 2.25 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

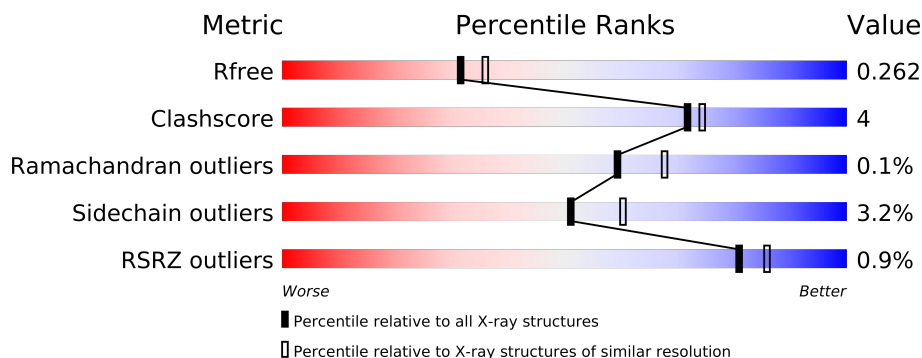
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.25 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}	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	217	
1	B	217	
1	C	217	
1	D	217	
1	E	217	
1	F	217	
1	G	217	
1	H	217	
1	I	217	
1	J	217	
2	K	13	
2	M	13	
2	O	13	
2	P	13	

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Mol	Chain	Length	Quality of chain
2	Q	13	
2	R	13	
2	S	13	
2	T	13	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18606 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SOLUBLE ACETYLCHOLINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	B	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	C	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	D	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	E	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	F	205	Total	C	N	O	S	0	1	0
			1640	1040	266	325	9			
1	G	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	H	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	I	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	J	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	VAL	ALA	CONFLICT	UNP Q8WSF8
A	136	VAL	ALA	CONFLICT	UNP Q8WSF8
B	41	VAL	ALA	CONFLICT	UNP Q8WSF8
B	136	VAL	ALA	CONFLICT	UNP Q8WSF8
C	41	VAL	ALA	CONFLICT	UNP Q8WSF8
C	136	VAL	ALA	CONFLICT	UNP Q8WSF8
D	41	VAL	ALA	CONFLICT	UNP Q8WSF8
D	136	VAL	ALA	CONFLICT	UNP Q8WSF8
E	41	VAL	ALA	CONFLICT	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	136	VAL	ALA	CONFLICT	UNP Q8WSF8
F	41	VAL	ALA	CONFLICT	UNP Q8WSF8
F	136	VAL	ALA	CONFLICT	UNP Q8WSF8
G	41	VAL	ALA	CONFLICT	UNP Q8WSF8
G	136	VAL	ALA	CONFLICT	UNP Q8WSF8
G	41	VAL	ALA	CONFLICT	UNP Q8WSF8
G	136	VAL	ALA	CONFLICT	UNP Q8WSF8
H	41	VAL	ALA	CONFLICT	UNP Q8WSF8
H	136	VAL	ALA	CONFLICT	UNP Q8WSF8
I	41	VAL	ALA	CONFLICT	UNP Q8WSF8
I	136	VAL	ALA	CONFLICT	UNP Q8WSF8

- Molecule 2 is a protein called ALPHA-CONOTOXIN IML.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	13	Total 91	C 52	N 20	O 15	S 4	0	0	1
2	M	13	Total 91	C 52	N 20	O 15	S 4	0	0	1
2	O	13	Total 91	C 52	N 20	O 15	S 4	0	0	1
2	P	13	Total 91	C 52	N 20	O 15	S 4	0	0	1
2	Q	13	Total 91	C 52	N 20	O 15	S 4	0	0	1
2	R	13	Total 91	C 52	N 20	O 15	S 4	0	0	1
2	S	13	Total 91	C 52	N 20	O 15	S 4	0	0	1
2	T	13	Total 91	C 52	N 20	O 15	S 4	0	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total 139	O 139	0	0
3	B	165	Total 165	O 165	0	0
3	C	173	Total 173	O 173	0	0
3	D	155	Total 155	O 155	0	0

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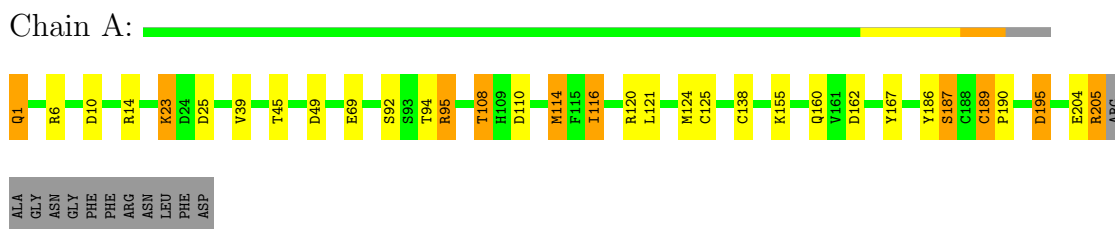
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	136	Total 136	O 136	0	0
3	F	136	Total 136	O 136	0	0
3	G	126	Total 126	O 126	0	0
3	H	128	Total 128	O 128	0	0
3	I	161	Total 161	O 161	0	0
3	J	157	Total 157	O 157	0	0
3	K	5	Total 5	O 5	0	0
3	M	4	Total 4	O 4	0	0
3	O	6	Total 6	O 6	0	0
3	P	2	Total 2	O 2	0	0
3	Q	3	Total 3	O 3	0	0
3	R	11	Total 11	O 11	0	0
3	S	2	Total 2	O 2	0	0
3	T	5	Total 5	O 5	0	0

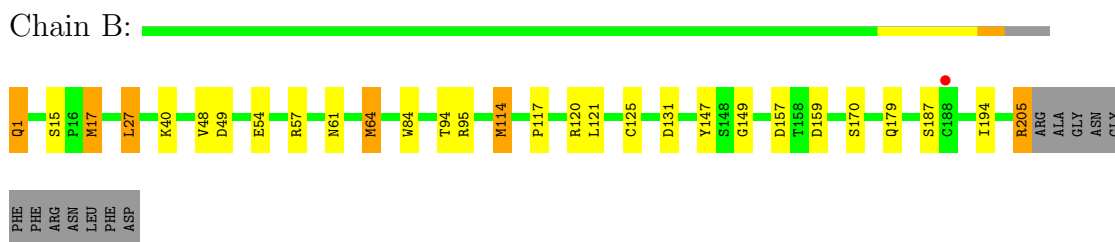
3 Residue-property plots

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.

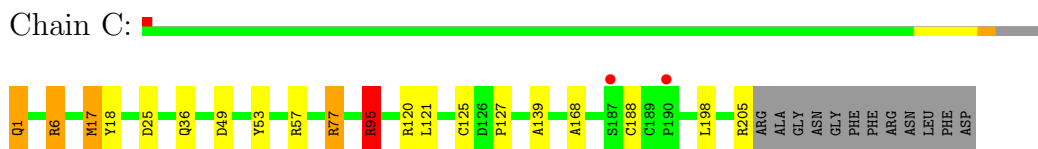
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



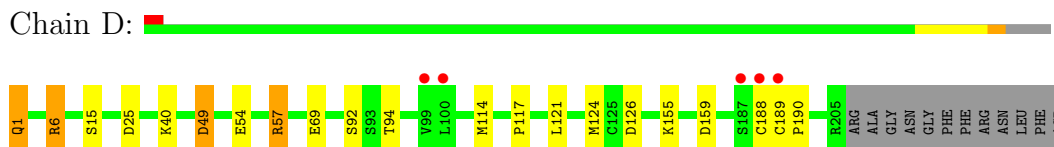
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



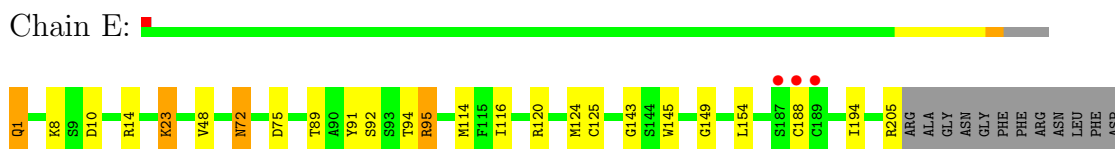
• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



• Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



- Molecule 2: ALPHA-CONOTOXIN IMI

Chain P:

There are no outlier residues recorded for this chain.

- Molecule 2: ALPHA-CONOTOXIN IMI

Chain Q:



- Molecule 2: ALPHA-CONOTOXIN IMI

Chain R:



- Molecule 2: ALPHA-CONOTOXIN IMI

Chain S:



- Molecule 2: ALPHA-CONOTOXIN IMI

Chain T:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.21Å 123.13Å 118.75Å 90.00° 117.47° 90.00°	Depositor
Resolution (Å)	105.41 – 2.25 54.05 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.1 (105.41-2.25) 96.8 (54.05-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.168 , 0.227 0.209 , 0.262	Depositor DCC
R_{free} test set	6659 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.5	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 132532 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18606	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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	0.89	4/1676 (0.2%)	0.91	7/2287 (0.3%)
1	B	0.84	0/1676	0.87	2/2287 (0.1%)
1	C	0.86	0/1676	0.85	2/2287 (0.1%)
1	D	0.83	0/1676	0.88	4/2287 (0.2%)
1	E	0.84	0/1676	0.84	1/2287 (0.0%)
1	F	0.86	4/1683 (0.2%)	0.89	3/2297 (0.1%)
1	G	0.83	1/1676 (0.1%)	0.88	2/2287 (0.1%)
1	H	0.81	0/1676	0.85	2/2287 (0.1%)
1	I	0.89	0/1676	0.93	2/2287 (0.1%)
1	J	0.88	0/1676	0.87	2/2287 (0.1%)
2	K	0.75	0/92	0.95	0/123
2	M	0.86	0/92	0.78	0/123
2	O	0.75	0/92	0.96	0/123
2	P	0.81	0/92	0.73	0/123
2	Q	0.76	0/92	0.71	0/123
2	R	0.83	0/92	0.79	0/123
2	S	0.90	0/92	0.83	0/123
2	T	0.94	0/92	1.03	0/123
All	All	0.85	9/17503 (0.1%)	0.88	27/23864 (0.1%)

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	C	0	1
1	D	0	1
1	E	0	1
1	H	0	1
1	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	186	TYR	C-N	-10.29	1.10	1.34
1	A	187	SER	C-N	-9.33	1.12	1.34
1	F	189	CYS	C-N	-9.24	1.16	1.34
1	A	190	PRO	C-N	-7.19	1.17	1.34
1	A	189	CYS	CB-SG	-6.36	1.71	1.82
1	F	77	ARG	CG-CD	-5.25	1.38	1.51
1	F	184	GLN	CD-OE1	5.14	1.35	1.24
1	G	140	VAL	CB-CG2	5.05	1.63	1.52
1	A	160	GLN	CD-OE1	5.02	1.34	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	6	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	G	6	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	F	6	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	H	6	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	J	6	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	I	6	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	I	6	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	B	27	LEU	CA-CB-CG	6.88	131.12	115.30
1	D	57	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	6	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	D	6	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	189	CYS	CA-CB-SG	6.13	125.04	114.00
1	F	6	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	F	189	CYS	O-C-N	-5.97	109.75	121.10
1	A	162	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	6	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	E	95	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	H	6	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	D	49	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	95	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	195	ASP	CB-CG-OD1	-5.56	113.29	118.30
1	A	186	TYR	O-C-N	5.39	131.33	122.70
1	G	6	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	6	ARG	NE-CZ-NH2	-5.21	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	D	126	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	205	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	188	CYS	Peptide
1	D	188	CYS	Peptide
1	E	188	CYS	Peptide
1	H	188	CYS	Peptide
1	J	188	CYS	Peptide

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1636	0	1572	22	0
1	B	1636	0	1572	18	0
1	C	1636	0	1572	14	0
1	D	1636	0	1572	11	0
1	E	1636	0	1572	22	0
1	F	1640	0	1580	16	0
1	G	1636	0	1572	14	0
1	H	1636	0	1572	7	0
1	I	1636	0	1572	17	0
1	J	1636	0	1572	14	0
2	K	91	0	78	1	0
2	M	91	0	78	0	0
2	O	91	0	78	1	0
2	P	91	0	78	0	0
2	Q	91	0	78	2	0
2	R	91	0	78	4	0
2	S	91	0	78	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	91	0	78	0	0
3	A	139	0	0	3	0
3	B	165	0	0	1	1
3	C	173	0	0	5	0
3	D	155	0	0	4	0
3	E	136	0	0	4	0
3	F	136	0	0	3	0
3	G	126	0	0	2	0
3	H	128	0	0	0	0
3	I	161	0	0	5	0
3	J	157	0	0	1	1
3	K	5	0	0	0	0
3	M	4	0	0	0	0
3	O	6	0	0	0	0
3	P	2	0	0	0	0
3	Q	3	0	0	1	0
3	R	11	0	0	1	0
3	S	2	0	0	0	0
3	T	5	0	0	0	0
All	All	18606	0	16352	145	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (145) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1:GLN:N	1:C:1:GLN:OE1	1.90	1.05
1:E:91:TYR:CE1	3:E:2075:HOH:O	2.14	1.01
1:B:1:GLN:N	1:B:1:GLN:OE1	1.91	1.01
1:D:1:GLN:OE1	1:D:1:GLN:HA	1.57	0.99
1:F:95:ARG:HD2	3:F:2044:HOH:O	1.64	0.98
1:G:1:GLN:OE1	1:G:1:GLN:N	1.98	0.96
1:A:1:GLN:N	1:A:1:GLN:OE1	2.00	0.94
1:A:114:MET:SD	1:A:116:ILE:CD1	2.59	0.91
1:F:1:GLN:N	1:F:1:GLN:OE1	2.05	0.89
1:A:69:GLU:HG2	3:I:2066:HOH:O	1.73	0.88
1:A:125:CYS:SG	1:A:138:CYS:CB	2.62	0.87
1:C:95:ARG:HD2	3:C:2053:HOH:O	1.73	0.86
1:A:114:MET:SD	1:A:116:ILE:HD13	2.19	0.83
1:J:1:GLN:N	1:J:1:GLN:CD	2.31	0.82
1:J:95:ARG:HD2	3:J:2093:HOH:O	1.84	0.76
1:A:114:MET:SD	1:A:116:ILE:HD11	2.25	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:1:GLN:H1	1:J:1:GLN:CD	1.88	0.76
1:J:114:MET:HE2	1:J:116:ILE:HD11	1.68	0.75
3:E:2054:HOH:O	1:J:69:GLU:HG2	1.90	0.71
1:J:57:ARG:HD2	1:J:113:VAL:O	1.91	0.71
3:D:2020:HOH:O	1:E:8:LYS:HE3	1.92	0.68
1:D:54:GLU:O	1:D:117:PRO:HD2	1.94	0.67
1:A:125:CYS:CB	1:A:138:CYS:SG	2.81	0.67
1:B:147:TYR:CE1	1:C:77:ARG:HD3	2.30	0.67
1:E:1:GLN:N	1:E:1:GLN:CD	2.51	0.64
1:D:6:ARG:NH2	1:D:69:GLU:O	2.31	0.64
1:G:48:VAL:HG21	1:G:125:CYS:SG	2.39	0.62
1:I:205:ARG:HE	1:I:205:ARG:C	2.02	0.62
1:E:10:ASP:HA	1:E:14:ARG:HD2	1.84	0.60
1:H:41:VAL:HG22	1:H:48:VAL:HG22	1.84	0.60
1:E:91:TYR:CZ	3:E:2075:HOH:O	2.41	0.59
1:D:25:ASP:CG	1:E:1:GLN:OE1	2.42	0.58
1:J:114:MET:CE	1:J:116:ILE:HD11	2.32	0.58
1:D:92:SER:HB2	1:D:124:MET:HE2	1.85	0.57
1:B:48:VAL:HG21	1:B:125:CYS:SG	2.44	0.57
1:H:48:VAL:HG21	1:H:125:CYS:SG	2.45	0.56
1:G:153:ASP:OD2	1:G:155:LYS:HE2	2.05	0.56
1:A:10:ASP:HA	1:A:14:ARG:HD2	1.88	0.56
1:E:1:GLN:H1	1:E:1:GLN:CD	2.07	0.56
1:G:41:VAL:HG13	1:G:127:PRO:HG3	1.89	0.55
1:B:57:ARG:NH2	1:B:157:ASP:OD2	2.40	0.55
1:C:6:ARG:HD3	3:C:2004:HOH:O	2.06	0.55
1:G:185:HIS:ND1	3:G:2117:HOH:O	2.33	0.55
1:E:23:LYS:NZ	1:E:23:LYS:HB3	2.21	0.55
2:R:8:CYS:O	2:R:11:ARG:HG3	2.07	0.55
1:I:54:GLU:O	1:I:117:PRO:HD2	2.07	0.55
1:D:94:THR:O	1:E:120:ARG:HD2	2.07	0.54
1:E:48:VAL:HG21	1:E:125:CYS:SG	2.47	0.54
1:E:92:SER:HB2	1:E:124:MET:HE2	1.89	0.54
1:I:69:GLU:CG	3:I:2065:HOH:O	2.56	0.53
1:F:92:SER:HB2	1:F:124:MET:HE2	1.91	0.53
1:J:1:GLN:H3	1:J:1:GLN:CD	2.10	0.53
2:Q:13:NH2:N	3:Q:2003:HOH:O	2.41	0.53
1:J:48:VAL:HG21	1:J:125:CYS:SG	2.49	0.53
3:D:2020:HOH:O	1:E:8:LYS:CE	2.55	0.52
1:A:92:SER:HB2	1:A:124:MET:HE2	1.91	0.52
1:G:95:ARG:NH2	3:G:2069:HOH:O	2.42	0.52
1:C:57:ARG:NH1	3:C:2068:HOH:O	2.42	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:114:MET:HE2	2:R:10:TRP:HA	1.91	0.51
1:F:17:MET:HE1	3:F:2064:HOH:O	2.11	0.51
1:C:139:ALA:HA	1:C:198:LEU:O	2.11	0.51
1:G:77:ARG:HG3	1:G:106:VAL:HG22	1.93	0.51
1:C:36:GLN:OE1	1:C:53:TYR:CE1	2.64	0.50
1:I:94:THR:O	1:J:120:ARG:HD2	2.12	0.50
1:I:173:GLU:HG2	1:I:205:ARG:HA	1.94	0.49
1:A:204:GLU:O	1:A:205:ARG:HG3	2.12	0.49
1:F:147:TYR:CE1	1:G:77:ARG:HD3	2.46	0.49
1:E:114:MET:HE2	1:E:116:ILE:HD11	1.93	0.49
1:G:154:LEU:HD13	1:G:196:VAL:HG23	1.93	0.49
1:F:94:THR:O	1:G:120:ARG:HD2	2.12	0.48
1:I:41:VAL:HG22	1:I:48:VAL:HG22	1.95	0.48
1:A:94:THR:O	1:B:120:ARG:HD2	2.14	0.48
1:D:155:LYS:HD3	3:D:2055:HOH:O	2.14	0.48
1:A:108:THR:HG22	1:A:110:ASP:OD1	2.14	0.48
1:G:41:VAL:HG22	1:G:48:VAL:HG22	1.96	0.47
1:B:147:TYR:CD1	1:C:77:ARG:HD3	2.49	0.47
1:B:54:GLU:O	1:B:117:PRO:HD2	2.15	0.47
1:E:114:MET:CE	1:E:116:ILE:HD11	2.45	0.46
1:A:167:TYR:HB2	1:E:124:MET:CE	2.45	0.46
1:C:168:ALA:O	1:C:205:ARG:NH2	2.49	0.46
1:F:6:ARG:HD3	3:F:2006:HOH:O	2.15	0.46
1:I:205:ARG:C	1:I:205:ARG:NE	2.69	0.46
1:D:57:ARG:HH11	1:D:114:MET:HB2	1.79	0.46
1:H:54:GLU:O	1:H:117:PRO:HD2	2.16	0.46
1:G:134:GLU:H	1:G:134:GLU:CD	2.18	0.45
1:H:114:MET:HG2	2:Q:10:TRP:HA	1.98	0.45
1:C:17:MET:HE2	1:C:18:TYR:H	1.81	0.45
1:F:120:ARG:HD2	1:J:94:THR:O	2.17	0.45
1:I:41:VAL:HG13	1:I:127:PRO:HG3	1.99	0.45
1:B:94:THR:O	1:C:120:ARG:HD2	2.17	0.45
1:C:125:CYS:O	1:C:127:PRO:HD3	2.16	0.45
1:B:17:MET:HE1	1:B:84:TRP:HB2	1.99	0.45
1:I:146:VAL:HB	1:J:77:ARG:HG2	1.99	0.45
1:I:147:TYR:CD1	1:J:77:ARG:HD3	2.52	0.45
1:A:49:ASP:HA	1:A:121:LEU:O	2.17	0.45
1:E:1:GLN:N	1:E:1:GLN:NE2	2.65	0.45
2:R:10:TRP:HD1	3:R:2008:HOH:O	1.99	0.45
1:F:48:VAL:HG21	1:F:125:CYS:SG	2.58	0.44
1:E:143:GLY:HA2	1:E:154:LEU:HD11	1.99	0.44
1:F:49:ASP:HA	1:F:121:LEU:O	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:6:ARG:NH2	1:F:69:GLU:O	2.35	0.44
1:B:170:SER:O	1:B:205:ARG:HD3	2.17	0.44
1:B:95:ARG:HD2	3:C:2102:HOH:O	2.16	0.44
1:B:61:ASN:O	1:B:64:MET:HG2	2.18	0.44
1:I:69:GLU:HG2	3:I:2065:HOH:O	2.18	0.43
1:A:45:THR:HG22	1:B:40:LYS:HB3	2.00	0.43
1:A:25:ASP:HB3	3:A:2016:HOH:O	2.18	0.43
2:R:2:CYS:O	2:R:8:CYS:HB3	2.18	0.43
1:I:69:GLU:HG3	3:I:2065:HOH:O	2.19	0.43
1:I:25:ASP:CG	1:I:25:ASP:O	2.56	0.43
1:A:120:ARG:HD2	1:E:94:THR:O	2.18	0.43
1:C:25:ASP:HB2	3:C:2009:HOH:O	2.17	0.43
1:A:10:ASP:O	1:A:14:ARG:HD3	2.19	0.43
1:B:149:GLY:HA3	1:B:194:ILE:CD1	2.49	0.43
1:G:139:ALA:HA	1:G:198:LEU:O	2.18	0.43
1:E:95:ARG:NE	3:E:2080:HOH:O	2.52	0.43
1:A:25:ASP:CB	3:A:2016:HOH:O	2.67	0.42
1:B:114:MET:HG2	3:B:2103:HOH:O	2.20	0.42
1:I:57:ARG:NH1	3:I:2057:HOH:O	2.52	0.42
1:H:147:TYR:CE1	1:I:77:ARG:HD3	2.54	0.42
1:I:136:VAL:O	1:I:201:LYS:HA	2.20	0.42
1:F:41:VAL:HG22	1:F:48:VAL:HG22	2.02	0.42
1:F:92:SER:CB	1:F:124:MET:HE2	2.50	0.42
1:H:6:ARG:NH2	1:H:69:GLU:O	2.42	0.42
1:E:145:TRP:O	2:O:6:PRO:HB2	2.20	0.42
1:G:49:ASP:HA	1:G:121:LEU:O	2.20	0.42
1:E:149:GLY:HA2	1:E:194:ILE:HD12	2.01	0.41
1:B:159:ASP:HA	1:B:179:GLN:O	2.20	0.41
1:B:49:ASP:HA	1:B:121:LEU:O	2.20	0.41
1:E:23:LYS:NZ	1:E:23:LYS:CB	2.82	0.41
1:H:182:GLN:OE1	1:H:195:ASP:OD2	2.38	0.41
1:A:92:SER:CB	1:A:124:MET:HE2	2.51	0.41
1:D:69:GLU:HG2	3:D:2065:HOH:O	2.20	0.41
2:S:2:CYS:O	2:S:8:CYS:HB3	2.21	0.41
1:F:205:ARG:C	1:F:205:ARG:HD2	2.41	0.41
1:B:149:GLY:CA	1:B:194:ILE:CD1	2.99	0.40
1:F:64:MET:HG2	1:F:110:ASP:C	2.42	0.40
1:A:23:LYS:NZ	1:A:23:LYS:HB3	2.36	0.40
1:D:189:CYS:HA	1:D:190:PRO:HD2	1.95	0.40
1:A:95:ARG:NE	3:A:2078:HOH:O	2.44	0.40
2:K:5:ASP:HA	2:K:6:PRO:HD2	1.95	0.40
1:D:49:ASP:HA	1:D:121:LEU:O	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:114:MET:HE3	1:J:116:ILE:HG12	2.04	0.40
1:C:49:ASP:HA	1:C:121:LEU:O	2.22	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	Distance(Å)	Clash(Å)
3:B:2129:HOH:O	3:J:2057:HOH:O[1_655]	2.17	0.03

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	203/217 (94%)	202 (100%)	1 (0%)	0	100	100
1	B	203/217 (94%)	196 (97%)	7 (3%)	0	100	100
1	C	203/217 (94%)	199 (98%)	4 (2%)	0	100	100
1	D	203/217 (94%)	201 (99%)	2 (1%)	0	100	100
1	E	203/217 (94%)	198 (98%)	4 (2%)	1 (0%)	38	38
1	F	204/217 (94%)	200 (98%)	3 (2%)	1 (0%)	38	38
1	G	203/217 (94%)	197 (97%)	6 (3%)	0	100	100
1	H	203/217 (94%)	200 (98%)	3 (2%)	0	100	100
1	I	203/217 (94%)	201 (99%)	2 (1%)	0	100	100
1	J	203/217 (94%)	200 (98%)	3 (2%)	0	100	100
2	K	11/13 (85%)	11 (100%)	0	0	100	100
2	M	11/13 (85%)	11 (100%)	0	0	100	100
2	O	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
2	P	11/13 (85%)	11 (100%)	0	0	100	100
2	Q	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
2	R	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
2	S	11/13 (85%)	10 (91%)	1 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	11/13 (85%)	11 (100%)	0	0	100	100
All	All	2119/2274 (93%)	2078 (98%)	39 (2%)	2 (0%)	59	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	187	SER
1	E	72	ASN

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	188/197 (95%)	177 (94%)	11 (6%)	28	27
1	B	188/197 (95%)	180 (96%)	8 (4%)	40	45
1	C	188/197 (95%)	184 (98%)	4 (2%)	66	75
1	D	188/197 (95%)	184 (98%)	4 (2%)	66	75
1	E	188/197 (95%)	182 (97%)	6 (3%)	51	60
1	F	189/197 (96%)	184 (97%)	5 (3%)	59	69
1	G	188/197 (95%)	180 (96%)	8 (4%)	40	45
1	H	188/197 (95%)	184 (98%)	4 (2%)	66	75
1	I	188/197 (95%)	185 (98%)	3 (2%)	75	84
1	J	188/197 (95%)	185 (98%)	3 (2%)	75	84
2	K	10/10 (100%)	9 (90%)	1 (10%)	11	7
2	M	10/10 (100%)	10 (100%)	0	100	100
2	O	10/10 (100%)	9 (90%)	1 (10%)	11	7
2	P	10/10 (100%)	10 (100%)	0	100	100
2	Q	10/10 (100%)	9 (90%)	1 (10%)	11	7
2	R	10/10 (100%)	9 (90%)	1 (10%)	11	7
2	S	10/10 (100%)	9 (90%)	1 (10%)	11	7
2	T	10/10 (100%)	9 (90%)	1 (10%)	11	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1961/2050 (96%)	1899 (97%)	62 (3%)	51 60

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	23	LYS
1	A	39	VAL
1	A	108	THR
1	A	114	MET
1	A	116	ILE
1	A	155	LYS
1	A	187	SER
1	A	189	CYS
1	A	195	ASP
1	A	205	ARG
1	B	1	GLN
1	B	15	SER
1	B	17	MET
1	B	27	LEU
1	B	64	MET
1	B	114	MET
1	B	131	ASP
1	B	187	SER
1	C	1	GLN
1	C	17	MET
1	C	77	ARG
1	C	95	ARG
1	D	1	GLN
1	D	15	SER
1	D	40	LYS
1	D	159	ASP
1	E	1	GLN
1	E	23	LYS
1	E	72	ASN
1	E	75	ASP
1	E	89	THR
1	E	205	ARG
1	F	15	SER
1	F	95	ARG
1	F	114	MET
1	F	158	THR

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Mol	Chain	Res	Type
1	F	188	CYS
1	G	1	GLN
1	G	36	GLN
1	G	77	ARG
1	G	131	ASP
1	G	133	GLU
1	G	134	GLU
1	G	187	SER
1	G	205	ARG
1	H	78	THR
1	H	114	MET
1	H	155	LYS
1	H	205	ARG
1	I	1	GLN
1	I	136	VAL
1	I	205	ARG
1	J	1	GLN
1	J	68	ASN
1	J	187	SER
2	K	11	ARG
2	O	4	SER
2	Q	4	SER
2	R	11	ARG
2	S	11	ARG
2	T	7	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	182	GLN
1	C	55	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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, 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	205/217 (94%)	-0.25	0 100 100	39, 45, 52, 60	0
1	B	205/217 (94%)	-0.16	1 (0%) 88 92	39, 46, 56, 62	0
1	C	205/217 (94%)	0.07	2 (0%) 79 84	37, 45, 53, 60	0
1	D	205/217 (94%)	0.14	5 (2%) 56 63	39, 45, 55, 63	0
1	E	205/217 (94%)	-0.12	3 (1%) 70 76	39, 45, 54, 60	0
1	F	205/217 (94%)	-0.15	5 (2%) 56 63	38, 45, 53, 60	0
1	G	205/217 (94%)	-0.12	2 (0%) 79 84	38, 45, 54, 58	0
1	H	205/217 (94%)	-0.08	0 100 100	39, 45, 52, 61	0
1	I	205/217 (94%)	0.13	0 100 100	40, 46, 53, 59	0
1	J	205/217 (94%)	-0.12	0 100 100	40, 45, 53, 62	0
2	K	13/13 (100%)	-0.62	0 100 100	33, 39, 48, 50	0
2	M	13/13 (100%)	0.34	1 (7%) 13 16	38, 43, 54, 54	0
2	O	13/13 (100%)	0.43	1 (7%) 13 16	39, 43, 55, 55	0
2	P	13/13 (100%)	0.37	0 100 100	40, 47, 54, 55	0
2	Q	13/13 (100%)	0.13	0 100 100	37, 48, 55, 55	0
2	R	13/13 (100%)	-0.30	0 100 100	30, 37, 46, 47	0
2	S	13/13 (100%)	-0.49	0 100 100	30, 38, 46, 49	0
2	T	13/13 (100%)	0.37	0 100 100	35, 39, 49, 51	0
All	All	2154/2274 (94%)	-0.06	20 (0%) 81 86	30, 45, 54, 63	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	188	CYS	3.5
1	F	187	SER	2.9
1	D	188	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	187	SER	2.7
1	F	188	CYS	2.6
1	G	187	SER	2.6
1	D	187	SER	2.5
1	D	189	CYS	2.5
1	F	133	GLU	2.4
1	G	188	CYS	2.4
2	M	12	CYS	2.4
1	C	190	PRO	2.3
2	O	12	CYS	2.2
1	B	188	CYS	2.2
1	D	99	VAL	2.1
1	F	190	PRO	2.1
1	F	68	ASN	2.1
1	E	189	CYS	2.1
1	C	187	SER	2.0
1	D	100	LEU	2.0

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.