



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2021 – 12:15 PM EDT

PDB ID : 3PMZ
Title : Crystal Structure of the Complex of Acetylcholine Binding Protein and d-tubocurarine
Authors : Talley, T.T.; Harel, M.; Yamauchi, J.G.; Radic, Z.; Hansen, S.; Huxford, T.; Taylor, P.W.
Deposited on : 2010-11-18
Resolution : 2.44 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.17.1
buster-report : 1.1.7 (2018)
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) : 2.17.1

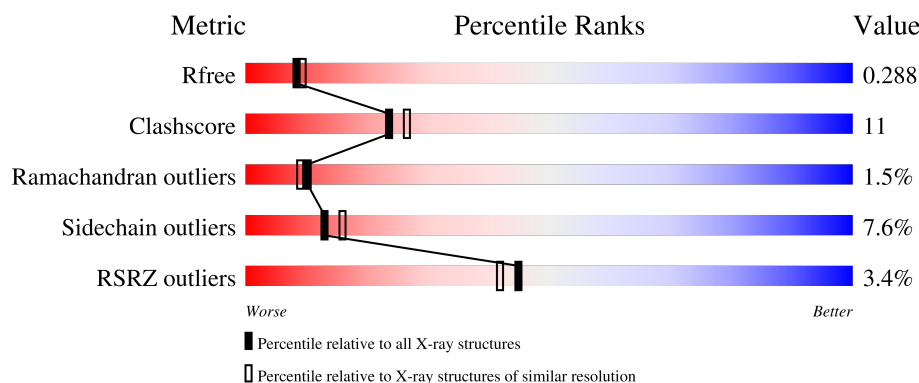
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

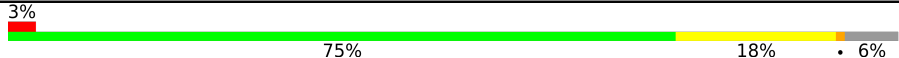
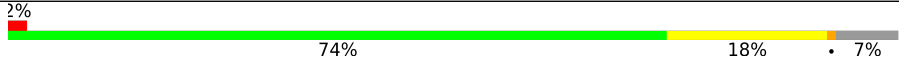



The reported resolution of this entry is 2.44 Å.

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}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	227	
1	B	227	
1	C	227	
1	D	227	
1	E	227	

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Mol	Chain	Length	Quality of chain
1	F	227	
1	G	227	
1	H	227	
1	I	227	
1	J	227	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	E	222	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17405 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1700	1071	280	340	9			
1	B	211	Total	C	N	O	S	0	0	0
			1685	1061	278	338	8			
1	C	215	Total	C	N	O	S	0	3	0
			1744	1099	290	346	9			
1	D	214	Total	C	N	O	S	0	2	0
			1725	1087	288	341	9			
1	E	211	Total	C	N	O	S	0	0	0
			1686	1064	278	335	9			
1	F	207	Total	C	N	O	S	0	0	0
			1648	1041	270	328	9			
1	G	211	Total	C	N	O	S	0	0	0
			1683	1061	276	338	8			
1	H	212	Total	C	N	O	S	0	0	0
			1693	1066	279	339	9			
1	I	212	Total	C	N	O	S	0	0	0
			1692	1067	279	337	9			
1	J	213	Total	C	N	O	S	0	0	0
			1697	1070	278	340	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP Q8WSF8
A	-6	TYR	-	expression tag	UNP Q8WSF8
A	-5	LYS	-	expression tag	UNP Q8WSF8
A	-4	ASP	-	expression tag	UNP Q8WSF8
A	-3	ASP	-	expression tag	UNP Q8WSF8
A	-2	ASP	-	expression tag	UNP Q8WSF8
A	-1	LYS	-	expression tag	UNP Q8WSF8
A	0	LEU	-	expression tag	UNP Q8WSF8
B	-7	ASP	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	TYR	-	expression tag	UNP Q8WSF8
B	-5	LYS	-	expression tag	UNP Q8WSF8
B	-4	ASP	-	expression tag	UNP Q8WSF8
B	-3	ASP	-	expression tag	UNP Q8WSF8
B	-2	ASP	-	expression tag	UNP Q8WSF8
B	-1	LYS	-	expression tag	UNP Q8WSF8
B	0	LEU	-	expression tag	UNP Q8WSF8
C	-7	ASP	-	expression tag	UNP Q8WSF8
C	-6	TYR	-	expression tag	UNP Q8WSF8
C	-5	LYS	-	expression tag	UNP Q8WSF8
C	-4	ASP	-	expression tag	UNP Q8WSF8
C	-3	ASP	-	expression tag	UNP Q8WSF8
C	-2	ASP	-	expression tag	UNP Q8WSF8
C	-1	LYS	-	expression tag	UNP Q8WSF8
C	0	LEU	-	expression tag	UNP Q8WSF8
D	-7	ASP	-	expression tag	UNP Q8WSF8
D	-6	TYR	-	expression tag	UNP Q8WSF8
D	-5	LYS	-	expression tag	UNP Q8WSF8
D	-4	ASP	-	expression tag	UNP Q8WSF8
D	-3	ASP	-	expression tag	UNP Q8WSF8
D	-2	ASP	-	expression tag	UNP Q8WSF8
D	-1	LYS	-	expression tag	UNP Q8WSF8
D	0	LEU	-	expression tag	UNP Q8WSF8
E	-7	ASP	-	expression tag	UNP Q8WSF8
E	-6	TYR	-	expression tag	UNP Q8WSF8
E	-5	LYS	-	expression tag	UNP Q8WSF8
E	-4	ASP	-	expression tag	UNP Q8WSF8
E	-3	ASP	-	expression tag	UNP Q8WSF8
E	-2	ASP	-	expression tag	UNP Q8WSF8
E	-1	LYS	-	expression tag	UNP Q8WSF8
E	0	LEU	-	expression tag	UNP Q8WSF8
F	-7	ASP	-	expression tag	UNP Q8WSF8
F	-6	TYR	-	expression tag	UNP Q8WSF8
F	-5	LYS	-	expression tag	UNP Q8WSF8
F	-4	ASP	-	expression tag	UNP Q8WSF8
F	-3	ASP	-	expression tag	UNP Q8WSF8
F	-2	ASP	-	expression tag	UNP Q8WSF8
F	-1	LYS	-	expression tag	UNP Q8WSF8
F	0	LEU	-	expression tag	UNP Q8WSF8
G	-7	ASP	-	expression tag	UNP Q8WSF8
G	-6	TYR	-	expression tag	UNP Q8WSF8
G	-5	LYS	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ASP	-	expression tag	UNP Q8WSF8
G	-3	ASP	-	expression tag	UNP Q8WSF8
G	-2	ASP	-	expression tag	UNP Q8WSF8
G	-1	LYS	-	expression tag	UNP Q8WSF8
G	0	LEU	-	expression tag	UNP Q8WSF8
H	-7	ASP	-	expression tag	UNP Q8WSF8
H	-6	TYR	-	expression tag	UNP Q8WSF8
H	-5	LYS	-	expression tag	UNP Q8WSF8
H	-4	ASP	-	expression tag	UNP Q8WSF8
H	-3	ASP	-	expression tag	UNP Q8WSF8
H	-2	ASP	-	expression tag	UNP Q8WSF8
H	-1	LYS	-	expression tag	UNP Q8WSF8
H	0	LEU	-	expression tag	UNP Q8WSF8
I	-7	ASP	-	expression tag	UNP Q8WSF8
I	-6	TYR	-	expression tag	UNP Q8WSF8
I	-5	LYS	-	expression tag	UNP Q8WSF8
I	-4	ASP	-	expression tag	UNP Q8WSF8
I	-3	ASP	-	expression tag	UNP Q8WSF8
I	-2	ASP	-	expression tag	UNP Q8WSF8
I	-1	LYS	-	expression tag	UNP Q8WSF8
I	0	LEU	-	expression tag	UNP Q8WSF8
J	-7	ASP	-	expression tag	UNP Q8WSF8
J	-6	TYR	-	expression tag	UNP Q8WSF8
J	-5	LYS	-	expression tag	UNP Q8WSF8
J	-4	ASP	-	expression tag	UNP Q8WSF8
J	-3	ASP	-	expression tag	UNP Q8WSF8
J	-2	ASP	-	expression tag	UNP Q8WSF8
J	-1	LYS	-	expression tag	UNP Q8WSF8
J	0	LEU	-	expression tag	UNP Q8WSF8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

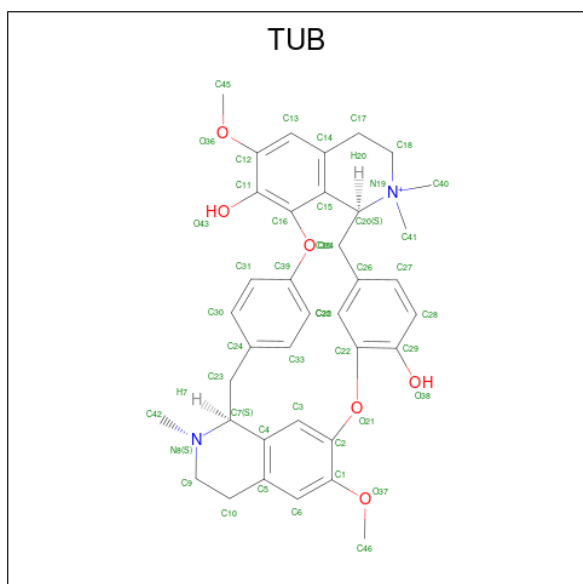
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	1	Total Mg 1 1	0	0
2	D	3	Total Mg 3 3	0	0
2	E	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	2	Total	Mg	0	0
			2	2		
2	G	1	Total	Mg	0	0
			1	1		
2	I	2	Total	Mg	0	0
			2	2		
2	J	1	Total	Mg	0	0
			1	1		

- Molecule 3 is (1beta,1'alpha)-7',12'-dihydroxy-6,6'-dimethoxy-2,2',2'-trimethyltubocuraran-2'-ium (three-letter code: TUB) (formula: C₃₇H₄₁N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			45	37	2	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	41	Total	O	0	0
			41	41		
4	C	57	Total	O	0	0
			57	57		
4	D	56	Total	O	0	0
			56	56		

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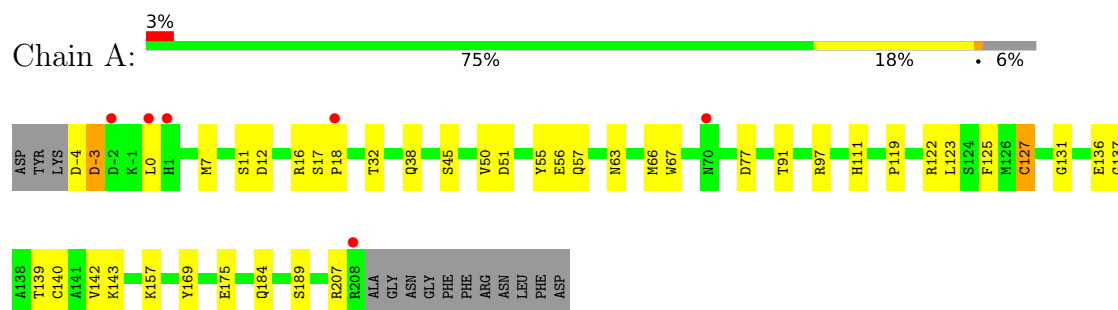
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	71	Total 71	O 71	0	0
4	F	22	Total 22	O 22	0	0
4	G	14	Total 14	O 14	0	0
4	H	11	Total 11	O 11	0	0
4	I	22	Total 22	O 22	0	0
4	J	39	Total 39	O 39	0	0

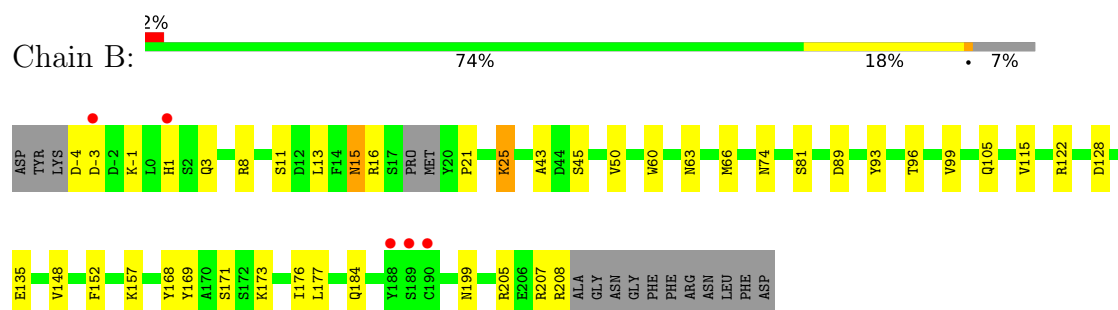
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

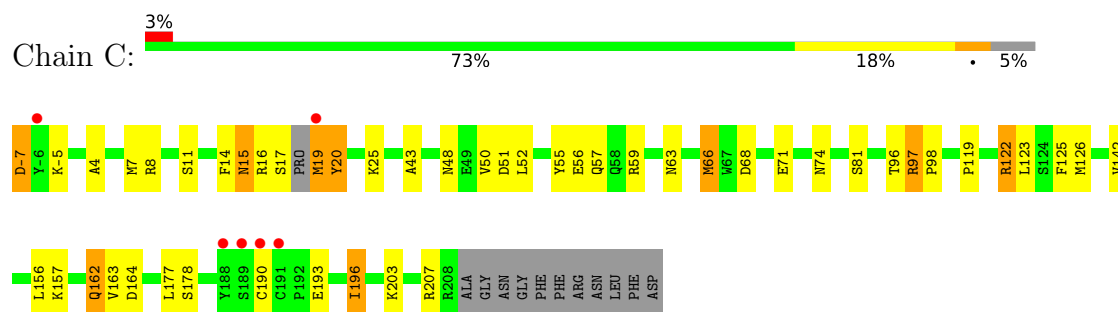
- Molecule 1: Soluble acetylcholine receptor



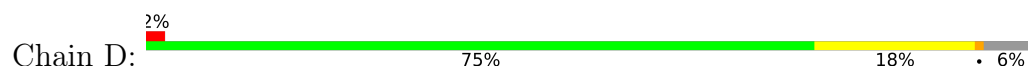
- Molecule 1: Soluble acetylcholine receptor

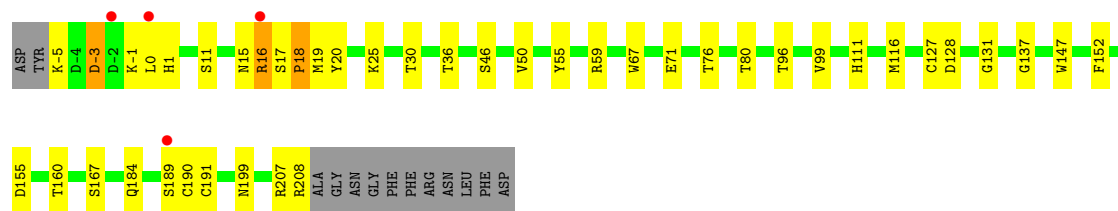


- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor





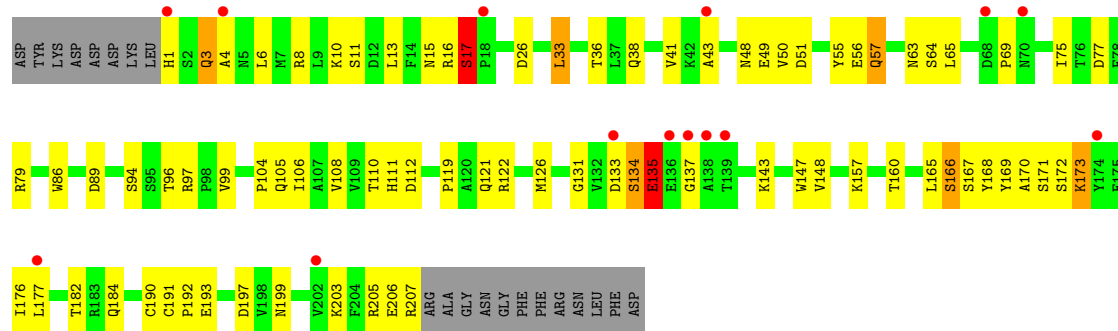
• Molecule 1: Soluble acetylcholine receptor

Chain E: 78% 13% 7%



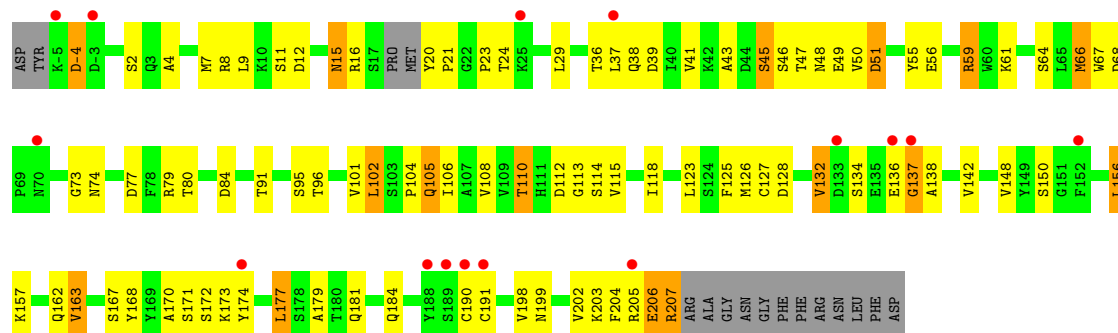
• Molecule 1: Soluble acetylcholine receptor

Chain F: 6% 56% 32% 9%



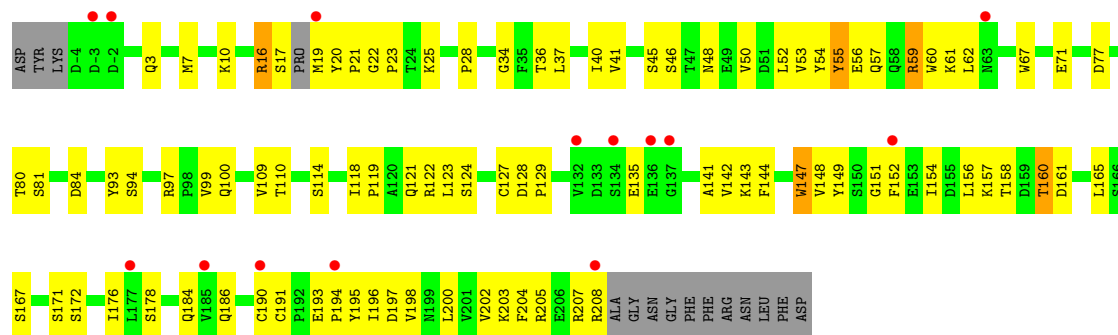
• Molecule 1: Soluble acetylcholine receptor

Chain G: 7% 51% 35% 7% 7%

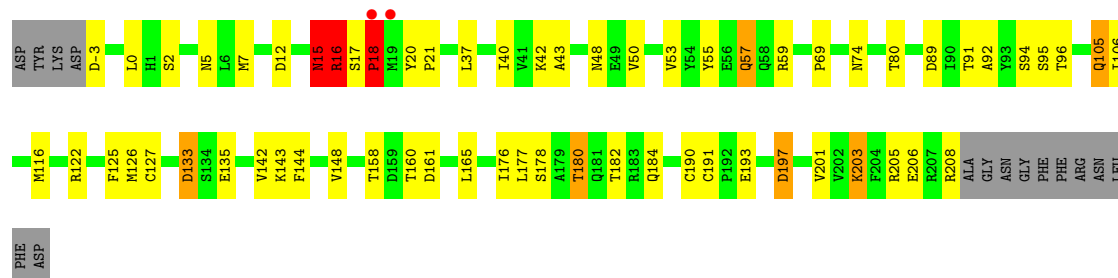


• Molecule 1: Soluble acetylcholine receptor

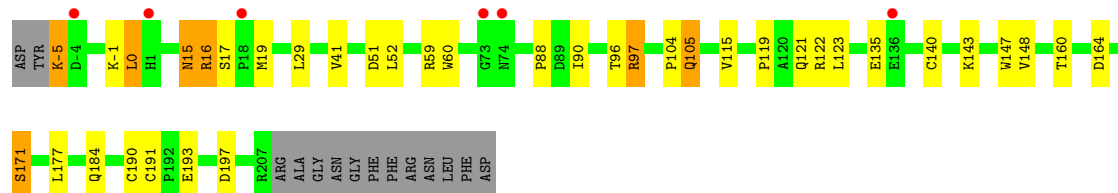
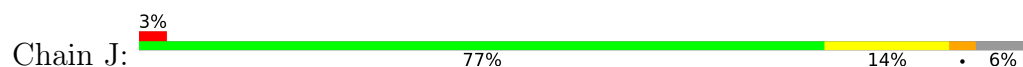
Chain H: 6% 52% 39% 7%



• Molecule 1: Soluble acetylcholine receptor



• Molecule 1: Soluble acetylcholine receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	142.74Å 194.04Å 101.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.71 – 2.44 48.51 – 2.44	Depositor EDS
% Data completeness (in resolution range)	96.8 (114.71-2.44) 96.8 (48.51-2.44)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.228 , 0.294 0.226 , 0.288	Depositor DCC
R_{free} test set	5105 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17405	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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

5.1 Standard geometry

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

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	0.88	1/1741 (0.1%)	0.87	2/2373 (0.1%)
1	B	0.84	0/1724	0.84	0/2348
1	C	0.94	0/1793	0.93	3/2439 (0.1%)
1	D	0.96	0/1772	0.93	1/2413 (0.0%)
1	E	0.93	0/1726	0.92	1/2350 (0.0%)
1	F	0.77	0/1689	0.86	0/2304
1	G	0.77	0/1722	0.85	2/2345 (0.1%)
1	H	0.76	0/1732	0.84	2/2358 (0.1%)
1	I	0.80	0/1733	0.79	0/2362
1	J	0.85	0/1736	0.89	5/2366 (0.2%)
All	All	0.85	1/17368 (0.0%)	0.87	16/23658 (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	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	CYS	CB-SG	5.07	1.90	1.82

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	0	LEU	CA-CB-CG	6.13	129.40	115.30
1	C	122	ARG	NE-CZ-NH1	5.74	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	195	TYR	N-CA-C	-5.67	95.70	111.00
1	A	97	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	G	51	ASP	CB-CG-OD1	5.51	123.26	118.30
1	G	68	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	164	ASP	CB-CG-OD1	5.36	123.12	118.30
1	J	52	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	0	LEU	CA-CB-CG	5.30	127.49	115.30
1	D	128	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	126	MET	CG-SD-CE	5.16	108.46	100.20
1	J	29	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	J	164	ASP	CB-CG-OD1	5.12	122.91	118.30
1	H	202	VAL	N-CA-C	5.11	124.81	111.00
1	E	133	ASP	CB-CG-OD1	5.05	122.85	118.30
1	J	140	CYS	CA-CB-SG	-5.00	105.00	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	17	SER	Peptide

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	1700	0	1625	20	0
1	B	1685	0	1608	24	0
1	C	1744	0	1677	41	0
1	D	1725	0	1664	32	0
1	E	1686	0	1616	22	0
1	F	1648	0	1576	60	0
1	G	1683	0	1608	75	0
1	H	1693	0	1617	69	0
1	I	1692	0	1621	49	0
1	J	1697	0	1616	32	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	1	0	0	0	0
2	I	2	0	0	0	0
2	J	1	0	0	0	0
3	E	45	0	40	6	0
4	A	58	0	0	0	0
4	B	41	0	0	0	0
4	C	57	0	0	0	0
4	D	56	0	0	1	0
4	E	71	0	0	0	0
4	F	22	0	0	0	0
4	G	14	0	0	2	0
4	H	11	0	0	0	0
4	I	22	0	0	2	0
4	J	39	0	0	0	0
All	All	17405	0	16268	374	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 11.

All (374) 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:F:184:GLN:NE2	1:F:199:ASN:HB2	1.56	1.19
1:I:59:ARG:HD3	1:I:116:MET:CE	1.85	1.06
1:F:173:LYS:HE3	1:G:45:SER:O	1.60	1.00
1:G:105:GLN:HE21	1:G:105:GLN:HA	1.30	0.97
1:F:38:GLN:HB3	1:G:126:MET:HE1	1.45	0.95
1:J:97:ARG:HG3	1:J:97:ARG:HH11	1.31	0.95
1:F:184:GLN:HE21	1:F:199:ASN:HB2	1.21	0.93
1:I:59:ARG:HD3	1:I:116:MET:HE1	1.46	0.93
1:J:177:LEU:CB	1:J:177:LEU:CD2	2.50	0.89
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.13	0.88
1:G:105:GLN:HA	1:G:105:GLN:NE2	1.83	0.87
1:I:180:THR:OG1	1:I:201:VAL:HB	1.74	0.87
1:J:177:LEU:CD2	1:J:177:LEU:CD1	2.53	0.86
1:J:177:LEU:CB	1:J:177:LEU:CD1	2.55	0.85
1:J:97:ARG:HH11	1:J:97:ARG:CG	1.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:SER:HB3	1:G:128:ASP:HB2	1.58	0.84
1:G:20:TYR:CD1	1:G:21:PRO:HD2	2.12	0.83
1:B:135:GLU:HB2	1:B:208:ARG:HH22	1.43	0.83
1:F:36:THR:HB	1:F:55:TYR:HB2	1.58	0.82
1:I:59:ARG:HD3	1:I:116:MET:HE2	1.61	0.81
1:F:41:VAL:CG1	1:G:49:GLU:OE2	2.29	0.80
1:G:79:ARG:HD2	1:G:108:VAL:HG22	1.62	0.80
1:F:33:LEU:HA	1:F:57:GLN:O	1.83	0.79
1:G:173:LYS:O	1:G:174:TYR:CD2	2.35	0.79
1:G:105:GLN:HE21	1:G:105:GLN:CA	1.95	0.78
1:F:43:ALA:HA	1:F:50:VAL:HG22	1.66	0.78
1:D:50:VAL:CG2	1:D:127:CYS:SG	2.72	0.78
1:F:134:SER:OG	1:F:135:GLU:N	2.16	0.77
1:I:57:GLN:HG2	4:I:230:HOH:O	1.83	0.77
1:G:172:SER:O	1:G:207:ARG:HD3	1.83	0.77
1:D:16:ARG:N	1:D:18:PRO:HD3	2.00	0.77
1:H:17:SER:HB3	1:H:19:MET:HG2	1.68	0.76
1:I:15:ASN:C	1:I:18:PRO:HD3	2.05	0.76
1:D:-5:LYS:N	4:D:299:HOH:O	2.18	0.76
1:E:143:LYS:HE3	1:E:184:GLN:HE22	1.49	0.76
1:H:178:SER:HB3	1:H:203:LYS:HB2	1.67	0.76
1:C:7:MET:HE1	1:D:17:SER:O	1.86	0.74
1:H:100:GLN:OE1	1:H:122:ARG:HD3	1.86	0.74
1:I:105:GLN:HA	1:I:105:GLN:HE21	1.51	0.74
1:F:192:PRO:HD2	1:F:193:GLU:OE1	1.89	0.73
1:G:184:GLN:NE2	1:G:199:ASN:HB2	2.04	0.73
1:F:110:THR:HG22	1:F:112:ASP:OD1	1.90	0.72
3:E:220:TUB:H35	3:E:220:TUB:C39	2.20	0.71
1:H:17:SER:O	1:H:19:MET:HB3	1.90	0.71
1:F:184:GLN:NE2	1:F:199:ASN:CB	2.45	0.71
1:C:8:ARG:HG2	1:I:16:ARG:HH22	1.56	0.70
1:F:41:VAL:HG11	1:G:49:GLU:OE2	1.89	0.70
1:F:171:SER:CB	1:G:128:ASP:HB2	2.21	0.70
1:D:-1:LYS:HD2	1:E:27:ASP:OD1	1.93	0.69
1:G:73:GLY:O	1:G:74:ASN:HB2	1.94	0.68
1:H:77:ASP:HB3	1:H:110:THR:HA	1.77	0.67
1:I:15:ASN:O	1:I:16:ARG:C	2.31	0.67
1:C:63:ASN:O	1:C:66:MET:HG2	1.94	0.67
1:F:3:GLN:HE22	1:G:20:TYR:HE1	1.43	0.67
1:B:63:ASN:O	1:B:66:MET:HG3	1.95	0.66
1:C:19:MET:O	1:C:20:TYR:C	2.33	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:GLN:NE2	1:G:105:GLN:CA	2.57	0.66
1:B:135:GLU:HB2	1:B:208:ARG:NH2	2.11	0.66
1:G:177:LEU:HD12	1:G:203:LYS:HB3	1.78	0.66
1:I:15:ASN:OD1	1:I:15:ASN:N	2.30	0.65
1:G:110:THR:HG22	1:G:112:ASP:OD1	1.98	0.64
1:D:15:ASN:HB2	1:D:16:ARG:HE	1.62	0.64
1:H:25:LYS:O	1:H:28:PRO:HD3	1.98	0.63
1:J:143:LYS:HE2	1:J:184:GLN:HE22	1.63	0.63
1:F:48:ASN:ND2	1:J:171:SER:O	2.31	0.62
1:B:8:ARG:HA	1:J:16:ARG:NH2	2.15	0.62
1:D:15:ASN:C	1:D:18:PRO:HD3	2.20	0.62
1:G:43:ALA:CB	1:G:174:TYR:OH	2.47	0.62
1:F:41:VAL:O	1:G:47:THR:HB	2.00	0.61
1:B:173:LYS:HD3	1:C:48:ASN:OD1	2.00	0.61
1:G:125:PHE:CD1	1:G:142:VAL:HB	2.35	0.61
1:C:15:ASN:N	1:C:15:ASN:HD22	1.97	0.61
1:H:142:VAL:HG12	1:H:200:LEU:HB3	1.81	0.61
1:C:19:MET:O	1:C:19:MET:HG3	2.00	0.61
1:E:207:ARG:O	1:E:208:ARG:HD2	2.01	0.60
1:F:168:TYR:CE1	1:F:176:ILE:HD11	2.37	0.60
1:C:15:ASN:N	1:C:15:ASN:ND2	2.49	0.60
1:J:97:ARG:HG3	1:J:97:ARG:NH1	2.03	0.60
1:I:133:ASP:HA	1:I:206:GLU:OE1	2.02	0.60
1:H:122:ARG:HD2	1:I:96:THR:O	2.01	0.60
1:F:69:PRO:HB3	1:F:75:ILE:O	2.02	0.60
1:J:184:GLN:NE2	1:J:197:ASP:OD1	2.33	0.59
1:J:15:ASN:O	1:J:16:ARG:HB2	2.01	0.59
1:E:89:ASP:OD2	1:E:148:VAL:HG22	2.03	0.58
1:J:-5:LYS:NZ	1:J:-5:LYS:HB3	2.18	0.58
1:F:3:GLN:O	1:F:6:LEU:N	2.36	0.58
1:I:50:VAL:HG21	1:I:127:CYS:SG	2.43	0.58
1:G:95:SER:N	4:G:228:HOH:O	2.37	0.58
1:H:61:LYS:HD2	1:H:114:SER:HB3	1.86	0.58
1:B:43:ALA:HA	1:B:50:VAL:HG22	1.86	0.57
1:G:43:ALA:HB2	1:G:174:TYR:OH	2.04	0.57
1:C:97[B]:ARG:HH11	1:C:97[B]:ARG:CG	2.16	0.57
1:G:61:LYS:HA	1:G:113:GLY:O	2.04	0.57
1:G:36:THR:HB	1:G:55:TYR:HB2	1.86	0.57
1:F:173:LYS:HG3	1:G:48:ASN:ND2	2.18	0.57
1:A:63:ASN:O	1:A:66:MET:HG3	2.04	0.57
1:E:16:ARG:NH2	1:G:8:ARG:HD3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:ARG:HD2	1:J:96:THR:O	2.04	0.57
1:B:11:SER:HA	1:B:15:ASN:HD21	1.69	0.56
1:I:50:VAL:HG23	1:I:127:CYS:HB3	1.87	0.56
1:A:131:GLY:O	1:A:137:GLY:HA2	2.05	0.56
1:F:86:TRP:O	1:F:86:TRP:CE3	2.58	0.56
1:G:38:GLN:O	1:G:39:ASP:HB2	2.05	0.56
1:C:7:MET:CE	1:D:17:SER:O	2.53	0.56
1:G:138:ALA:O	1:G:203:LYS:HA	2.06	0.56
1:C:122:ARG:HD2	1:D:96:THR:O	2.05	0.56
1:D:15:ASN:HA	1:D:18:PRO:HD3	1.85	0.56
1:I:40:ILE:HD11	1:I:176:ILE:HD11	1.88	0.56
1:H:52:LEU:O	1:H:122:ARG:HA	2.05	0.56
1:J:105:GLN:HE21	1:J:105:GLN:HA	1.72	0.55
1:F:105:GLN:HE21	1:F:105:GLN:HA	1.72	0.55
1:H:17:SER:C	1:H:19:MET:HB3	2.26	0.55
1:A:56:GLU:O	1:A:119:PRO:HD2	2.06	0.55
1:D:67:TRP:CZ3	1:D:111:HIS:HA	2.42	0.55
1:I:50:VAL:CG2	1:I:127:CYS:SG	2.94	0.55
1:I:177:LEU:HB2	1:I:203:LYS:HB3	1.88	0.55
1:C:43:ALA:HA	1:C:50:VAL:HG22	1.89	0.55
1:D:50:VAL:HG23	1:D:127:CYS:HB3	1.87	0.55
1:F:171:SER:O	1:G:48:ASN:ND2	2.40	0.55
1:G:173:LYS:HG3	1:H:48:ASN:ND2	2.22	0.55
1:F:173:LYS:CE	1:G:45:SER:O	2.46	0.55
1:G:95:SER:CB	1:G:123:LEU:HD11	2.37	0.54
1:B:169:TYR:CZ	1:B:171:SER:HB2	2.42	0.54
1:F:165:LEU:O	1:F:167:SER:N	2.39	0.54
1:H:36:THR:O	1:H:54:TYR:CB	2.56	0.54
1:D:15:ASN:CA	1:D:18:PRO:HD3	2.37	0.54
1:H:36:THR:O	1:H:54:TYR:HB2	2.07	0.54
1:F:51:ASP:HB3	1:F:122:ARG:HE	1.72	0.54
1:H:93:TYR:HD2	1:H:143:LYS:HB2	1.73	0.54
1:F:99:VAL:HG12	1:F:121:GLN:HB3	1.89	0.54
1:G:51:ASP:HA	1:G:123:LEU:O	2.08	0.54
1:B:-1:LYS:O	1:B:3:GLN:HB2	2.09	0.53
1:G:66:MET:SD	1:G:112:ASP:O	2.65	0.53
1:H:80:THR:OG1	1:H:84:ASP:OD2	2.26	0.53
1:J:105:GLN:HA	1:J:105:GLN:NE2	2.22	0.53
1:G:-4:ASP:N	1:G:-4:ASP:OD1	2.41	0.53
1:E:172:SER:O	1:E:207:ARG:HD3	2.08	0.53
1:H:16:ARG:O	1:H:17:SER:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:119:PRO:HG2	1:J:121:GLN:HE21	1.74	0.53
1:G:173:LYS:C	1:G:174:TYR:CD2	2.82	0.53
1:H:3:GLN:O	1:H:7:MET:HG3	2.09	0.53
1:D:17:SER:O	1:D:18:PRO:O	2.27	0.53
1:E:24:THR:HG22	1:E:26:ASP:N	2.24	0.53
3:E:220:TUB:H35	3:E:220:TUB:O34	2.07	0.53
1:B:60:TRP:CZ2	1:B:115:VAL:HG11	2.44	0.52
1:D:50:VAL:HG23	1:D:127:CYS:SG	2.47	0.52
1:H:172:SER:O	1:H:207:ARG:HD3	2.10	0.52
1:C:63:ASN:O	1:C:66:MET:CG	2.57	0.52
1:C:55:TYR:CE2	1:D:147:TRP:HH2	2.27	0.52
1:C:-7:ASP:HB2	1:C:-5:LYS:H	1.74	0.52
1:G:106:ILE:HG21	1:H:148:VAL:HG21	1.92	0.52
1:E:29:LEU:C	1:E:29:LEU:HD23	2.30	0.52
1:F:168:TYR:CZ	1:F:176:ILE:HD11	2.45	0.52
1:I:143:LYS:NZ	1:I:184:GLN:HE22	2.06	0.52
1:F:135:GLU:HA	1:F:205:ARG:HD3	1.91	0.51
1:J:51:ASP:HA	1:J:123:LEU:O	2.11	0.51
1:I:42:LYS:HG3	1:I:43:ALA:N	2.24	0.51
1:I:105:GLN:HA	1:I:105:GLN:NE2	2.22	0.51
1:G:95:SER:HB3	1:G:123:LEU:HD11	1.93	0.51
1:I:40:ILE:CD1	1:I:176:ILE:HD11	2.40	0.51
1:H:204:PHE:N	1:H:204:PHE:CD2	2.77	0.51
1:C:16[B]:ARG:HH22	1:I:7:MET:HB3	1.76	0.51
1:D:36:THR:HB	1:D:55:TYR:HB2	1.93	0.51
1:F:89:ASP:OD2	1:F:148:VAL:HG22	2.11	0.51
1:H:7:MET:HG2	4:I:357:HOH:O	2.09	0.51
1:I:135:GLU:HG2	1:I:208:ARG:HH22	1.76	0.51
1:C:8:ARG:HD3	1:I:12:ASP:OD2	2.11	0.51
1:G:4:ALA:HA	1:G:7:MET:CE	2.41	0.51
1:G:43:ALA:HB3	1:G:174:TYR:OH	2.11	0.51
1:H:77:ASP:HB2	1:H:109:VAL:O	2.11	0.51
1:I:105:GLN:HE21	1:I:105:GLN:CA	2.22	0.51
1:H:157:LYS:HG3	1:H:158:THR:N	2.26	0.50
1:H:165:LEU:HD13	1:H:176:ILE:HG21	1.92	0.50
1:C:16[A]:ARG:NH2	1:I:16:ARG:HE	2.10	0.50
3:E:220:TUB:C24	3:E:220:TUB:C3	2.89	0.50
1:G:80:THR:OG1	1:G:84:ASP:OD2	2.28	0.50
1:H:54:TYR:OH	1:H:123:LEU:HD22	2.12	0.50
1:C:97[B]:ARG:HH11	1:C:97[B]:ARG:HG2	1.77	0.50
1:D:55:TYR:CE2	1:E:147:TRP:HH2	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:VAL:C	1:G:102:LEU:HD23	2.32	0.50
1:G:173:LYS:HD2	1:H:45:SER:O	2.12	0.50
1:B:25:LYS:HG2	1:B:152:PHE:HB3	1.92	0.50
1:A:125:PHE:CD1	1:A:142:VAL:HB	2.47	0.49
1:F:38:GLN:CB	1:G:126:MET:HE1	2.32	0.49
1:I:20:TYR:CD2	1:I:21:PRO:HD2	2.46	0.49
1:I:55:TYR:CE2	1:J:147:TRP:HH2	2.30	0.49
1:A:45:SER:O	1:E:173:LYS:CE	2.60	0.49
1:F:41:VAL:HG13	1:G:49:GLU:OE2	2.12	0.49
1:C:178:SER:OG	1:C:203:LYS:HG3	2.13	0.49
1:F:122:ARG:HD2	1:G:96:THR:O	2.13	0.49
1:A:45:SER:O	1:E:173:LYS:HE2	2.12	0.49
1:H:23:PRO:HD2	1:H:149:TYR:CZ	2.47	0.49
1:G:156:LEU:HD22	1:G:198:VAL:HG23	1.94	0.48
1:F:110:THR:O	1:F:112:ASP:N	2.46	0.48
1:J:191:CYS:HB3	1:J:193:GLU:OE2	2.13	0.48
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.54	0.48
1:I:178:SER:OG	1:I:203:LYS:HB2	2.13	0.48
1:J:-5:LYS:HB3	1:J:-5:LYS:HZ2	1.78	0.48
1:J:190:CYS:C	1:J:191:CYS:SG	2.92	0.48
1:H:16:ARG:O	1:H:17:SER:HB2	2.14	0.48
1:A:51:ASP:HA	1:A:123:LEU:O	2.14	0.48
1:C:68:ASP:HB3	1:C:71:GLU:HG3	1.95	0.48
1:C:59:ARG:HD3	1:C:59:ARG:C	2.35	0.48
1:G:205:ARG:HG2	1:G:206:GLU:O	2.13	0.47
1:H:56:GLU:O	1:H:56:GLU:HG2	2.14	0.47
1:J:41:VAL:HG11	1:J:122:ARG:HH12	1.79	0.47
1:A:38:GLN:OE1	1:A:55:TYR:CE2	2.68	0.47
3:E:220:TUB:C3	3:E:220:TUB:C33	2.92	0.47
1:G:23:PRO:HB3	1:G:29:LEU:HD23	1.97	0.47
1:B:184:GLN:NE2	1:B:199:ASN:HB2	2.29	0.47
1:F:177:LEU:HD11	1:F:205:ARG:HG2	1.96	0.47
1:J:97:ARG:CG	1:J:97:ARG:NH1	2.59	0.47
1:E:24:THR:CG2	1:E:26:ASP:H	2.27	0.47
1:G:137:GLY:HA3	1:G:204:PHE:O	2.15	0.47
1:J:41:VAL:HG11	1:J:122:ARG:NH1	2.30	0.47
1:F:86:TRP:O	1:F:86:TRP:HE3	1.98	0.47
1:G:11:SER:HA	1:G:15:ASN:HD21	1.80	0.47
1:F:133:ASP:HA	1:F:206:GLU:HG3	1.97	0.47
1:H:141:ALA:HA	1:H:200:LEU:O	2.15	0.47
1:H:144:PHE:N	1:H:198:VAL:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:GLU:HA	1:H:71:GLU:HA	1.96	0.46
1:B:13:LEU:HD23	1:B:13:LEU:HA	1.78	0.46
1:F:49:GLU:OE2	1:F:96:THR:OG1	2.29	0.46
1:E:151:GLY:HA2	1:E:154:ILE:O	2.16	0.46
1:I:69:PRO:O	1:I:74:ASN:HA	2.15	0.46
1:C:8:ARG:HG2	1:I:16:ARG:NH2	2.27	0.46
1:C:19:MET:O	1:C:20:TYR:O	2.33	0.46
1:G:170:ALA:N	4:G:230:HOH:O	2.45	0.46
1:F:96:THR:CG2	1:F:126:MET:HG3	2.46	0.46
1:C:177:LEU:HB2	1:C:203:LYS:HB2	1.98	0.46
1:G:56:GLU:O	1:G:118:ILE:HA	2.16	0.46
1:G:59:ARG:HA	1:G:115:VAL:O	2.16	0.46
1:F:106:ILE:HG21	1:G:148:VAL:HG21	1.98	0.45
1:H:48:ASN:OD1	1:H:128:ASP:HA	2.16	0.45
1:A:12:ASP:OD2	1:F:8:ARG:HD2	2.16	0.45
1:D:131:GLY:O	1:D:137:GLY:HA2	2.16	0.45
1:H:142:VAL:O	1:H:200:LEU:N	2.28	0.45
1:H:184:GLN:HB2	1:H:197:ASP:OD2	2.16	0.45
1:A:45:SER:O	1:E:173:LYS:NZ	2.49	0.45
1:H:20:TYR:CZ	1:H:62:LEU:HD22	2.52	0.45
1:H:37:LEU:HD11	1:H:52:LEU:HD22	1.98	0.45
1:I:190:CYS:C	1:I:191:CYS:SG	2.95	0.45
1:C:51:ASP:HA	1:C:123:LEU:O	2.17	0.45
1:F:165:LEU:C	1:F:167:SER:H	2.20	0.45
1:G:9:LEU:HD21	1:G:67:TRP:CE2	2.52	0.45
1:I:12:ASP:OD1	1:I:16:ARG:NH2	2.50	0.45
1:H:50:VAL:HB	1:H:127:CYS:HB3	1.99	0.44
1:J:15:ASN:O	1:J:16:ARG:CB	2.66	0.44
1:B:122:ARG:HD2	1:C:96:THR:O	2.16	0.44
1:A:7:MET:CE	1:B:21:PRO:HD3	2.47	0.44
1:H:20:TYR:HA	1:H:21:PRO:HD3	1.70	0.44
1:I:15:ASN:O	1:I:16:ARG:O	2.35	0.44
1:H:118:ILE:HG22	1:H:118:ILE:O	2.18	0.44
1:G:36:THR:O	1:G:36:THR:HG22	2.18	0.44
1:G:79:ARG:N	1:G:79:ARG:HD3	2.33	0.44
1:G:106:ILE:CG2	1:H:148:VAL:HG21	2.47	0.44
1:H:59:ARG:HH21	1:H:60:TRP:N	2.16	0.44
1:J:16:ARG:HG2	1:J:16:ARG:HH11	1.82	0.44
1:G:4:ALA:HA	1:G:7:MET:HE3	2.00	0.44
1:D:59:ARG:HD3	1:D:116:MET:CE	2.48	0.44
1:E:61:LYS:HA	1:E:114:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:TRP:O	3:E:220:TUB:H18	2.18	0.44
1:F:99:VAL:CG1	1:F:121:GLN:HB3	2.48	0.43
1:F:170:ALA:C	1:F:172:SER:H	2.21	0.43
1:I:37:LEU:HD12	1:I:53:VAL:O	2.18	0.43
1:I:125:PHE:CD1	1:I:142:VAL:HB	2.53	0.43
1:B:168:TYR:CE1	1:B:176:ILE:HD11	2.51	0.43
1:C:97[B]:ARG:CG	1:C:97[B]:ARG:NH1	2.79	0.43
1:B:11:SER:O	1:B:15:ASN:ND2	2.51	0.43
1:E:192:PRO:HD2	1:E:193:GLU:OE1	2.18	0.43
1:H:55:TYR:N	1:H:55:TYR:CD2	2.84	0.43
1:C:97[A]:ARG:HB2	1:C:98:PRO:CD	2.49	0.43
1:F:96:THR:O	1:F:97:ARG:HD3	2.19	0.43
1:H:128:ASP:HA	1:H:129:PRO:HD3	1.88	0.43
1:C:162[A]:GLN:HE21	1:C:163:VAL:N	2.17	0.43
1:D:184:GLN:NE2	1:D:199:ASN:HB2	2.34	0.43
1:C:4:ALA:O	1:C:8:ARG:HB2	2.19	0.43
1:C:162[A]:GLN:HE21	1:C:162[A]:GLN:CA	2.32	0.43
1:E:141:ALA:HA	1:E:200:LEU:O	2.19	0.43
1:E:193:GLU:CD	1:E:193:GLU:H	2.22	0.43
1:A:67:TRP:CZ3	1:A:111:HIS:HA	2.54	0.43
1:G:50:VAL:CG2	1:G:127:CYS:SG	3.07	0.43
1:I:158:THR:HB	1:I:160:THR:O	2.19	0.43
1:D:50:VAL:HG23	1:D:127:CYS:CB	2.48	0.43
1:A:143:LYS:HD3	1:A:184:GLN:HE22	1.84	0.42
1:A:169:TYR:OH	1:B:128:ASP:N	2.52	0.42
1:G:156:LEU:O	1:G:157:LYS:HB3	2.18	0.42
1:H:178:SER:HB3	1:H:203:LYS:HD2	2.00	0.42
1:J:-5:LYS:HD2	1:J:-5:LYS:O	2.18	0.42
1:D:16:ARG:H	1:D:18:PRO:HD3	1.83	0.42
1:F:169:TYR:CZ	1:F:171:SER:HB2	2.54	0.42
1:F:143:LYS:HB3	1:F:197:ASP:OD1	2.19	0.42
1:H:67:TRP:HH2	1:H:77:ASP:HA	1.84	0.42
1:A:77:ASP:C	1:A:77:ASP:OD1	2.57	0.42
1:A:139:THR:O	1:A:140:CYS:SG	2.77	0.42
1:C:52:LEU:HG	1:C:125:PHE:HE2	1.85	0.42
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.59	0.42
1:F:63:ASN:C	1:F:65:LEU:H	2.22	0.42
1:G:12:ASP:HA	1:G:16:ARG:HB2	2.01	0.42
1:H:178:SER:HB3	1:H:203:LYS:CD	2.49	0.42
1:H:20:TYR:CE2	1:H:62:LEU:HD22	2.54	0.42
1:H:151:GLY:HA2	1:H:154:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:PHE:C	1:C:15:ASN:HD22	2.23	0.42
1:E:139:THR:OG1	1:E:203:LYS:HG2	2.19	0.42
1:H:80:THR:O	1:H:81:SER:C	2.57	0.42
1:H:149:TYR:HB2	1:H:154:ILE:HD12	2.02	0.42
1:I:16:ARG:HA	1:I:17:SER:HA	1.87	0.42
1:F:79:ARG:HG3	1:F:108:VAL:HG22	2.02	0.42
1:F:190:CYS:SG	1:F:191:CYS:N	2.93	0.42
1:H:186:GLN:O	1:H:186:GLN:HG3	2.19	0.42
1:G:4:ALA:HA	1:G:7:MET:HE2	2.02	0.42
1:B:89:ASP:OD2	1:B:148:VAL:HG22	2.20	0.42
1:F:96:THR:O	1:J:122:ARG:HD2	2.20	0.42
1:G:95:SER:HB2	1:G:123:LEU:HD11	2.00	0.42
1:H:171:SER:O	1:I:48:ASN:ND2	2.45	0.42
1:F:10:LYS:O	1:F:11:SER:C	2.58	0.41
1:H:99:VAL:HG21	1:H:121:GLN:OE1	2.20	0.41
1:I:165:LEU:HD22	1:I:176:ILE:HG21	2.02	0.41
1:A:55:TYR:OH	1:B:93:TYR:O	2.37	0.41
1:G:50:VAL:HG23	1:G:127:CYS:HB3	2.02	0.41
1:I:2:SER:HA	1:I:5:ASN:HD22	1.85	0.41
1:G:79:ARG:HG2	1:H:149:TYR:CE1	2.55	0.41
1:J:88:PRO:HB2	1:J:90:ILE:HG12	2.02	0.41
1:D:25:LYS:HG3	1:D:152:PHE:HB3	2.01	0.41
1:E:129:PRO:O	1:E:132:VAL:HB	2.21	0.41
1:H:94:SER:OG	1:H:142:VAL:HG23	2.20	0.41
1:I:106:ILE:HG21	1:J:148:VAL:HG21	2.02	0.41
1:D:15:ASN:HB2	1:D:16:ARG:NE	2.34	0.41
1:F:56:GLU:O	1:F:119:PRO:HD2	2.20	0.41
1:G:50:VAL:HG21	1:G:127:CYS:SG	2.61	0.41
1:G:104:PRO:HG2	1:H:147:TRP:HB2	2.02	0.41
1:G:163:VAL:HB	1:G:179:ALA:HB1	2.03	0.41
1:G:181:GLN:HA	1:G:199:ASN:O	2.21	0.41
1:H:10:LYS:HE3	1:H:10:LYS:HB3	1.85	0.41
1:H:53:VAL:HG11	1:I:126:MET:HE1	2.02	0.41
1:C:156:LEU:H	1:C:196:ILE:HG21	1.86	0.41
1:D:-3:ASP:O	1:D:1:HIS:CD2	2.74	0.41
1:D:59:ARG:HD3	1:D:116:MET:HE3	2.02	0.41
3:E:220:TUB:O34	3:E:220:TUB:C35	2.67	0.41
1:H:196:ILE:HG13	1:H:197:ASP:H	1.85	0.41
1:A:32:THR:HA	1:A:157:LYS:O	2.19	0.41
1:B:105:GLN:NE2	1:B:105:GLN:HA	2.35	0.41
1:H:19:MET:O	1:H:19:MET:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:PHE:CD1	1:C:142:VAL:HB	2.56	0.41
1:H:20:TYR:CZ	1:H:22:GLY:O	2.73	0.41
1:H:119:PRO:HG2	1:H:121:GLN:HE21	1.85	0.41
1:I:92:ALA:HB2	1:I:144:PHE:CE1	2.56	0.41
1:J:60:TRP:CZ2	1:J:115:VAL:HG11	2.56	0.41
1:A:122:ARG:HD2	1:B:96:THR:O	2.20	0.41
1:B:25:LYS:HE2	1:B:152:PHE:HB3	2.03	0.41
1:B:177:LEU:HD21	1:B:205:ARG:HD3	2.03	0.41
1:F:147:TRP:CB	1:J:104:PRO:HG2	2.50	0.41
1:G:162:GLN:O	1:G:163:VAL:C	2.60	0.41
1:H:160:THR:OG1	1:H:161:ASP:N	2.53	0.41
1:I:59:ARG:CD	1:I:116:MET:HE2	2.42	0.41
1:F:106:ILE:CG2	1:G:148:VAL:HG21	2.50	0.41
1:F:10:LYS:O	1:F:13:LEU:N	2.53	0.40
1:F:131:GLY:O	1:F:137:GLY:C	2.59	0.40
1:H:142:VAL:CG1	1:H:200:LEU:HB3	2.49	0.40
1:F:16:ARG:HA	1:F:17:SER:HA	1.52	0.40
1:H:41:VAL:HG11	1:H:122:ARG:HH12	1.86	0.40
1:I:16:ARG:N	1:I:18:PRO:HD3	2.35	0.40
1:D:16:ARG:HA	1:D:17:SER:HA	1.81	0.40
1:D:190:CYS:SG	1:D:191:CYS:N	2.94	0.40
1:H:190:CYS:C	1:H:191:CYS:SG	3.00	0.40
1:C:11:SER:O	1:C:16[A]:ARG:HD2	2.21	0.40
1:C:56:GLU:O	1:C:119:PRO:HD2	2.21	0.40
1:D:30:THR:HA	1:D:155:ASP:O	2.21	0.40
1:H:196:ILE:HG13	1:H:197:ASP:N	2.36	0.40
1:I:89:ASP:OD2	1:I:148:VAL:HG22	2.21	0.40
1:I:184:GLN:HE21	1:I:197:ASP:CG	2.23	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	211/227 (93%)	202 (96%)	6 (3%)	3 (1%)	11	10
1	B	207/227 (91%)	201 (97%)	6 (3%)	0	100	100
1	C	214/227 (94%)	204 (95%)	8 (4%)	2 (1%)	17	20
1	D	214/227 (94%)	206 (96%)	6 (3%)	2 (1%)	17	20
1	E	207/227 (91%)	201 (97%)	6 (3%)	0	100	100
1	F	205/227 (90%)	178 (87%)	18 (9%)	9 (4%)	2	0
1	G	207/227 (91%)	174 (84%)	25 (12%)	8 (4%)	3	1
1	H	208/227 (92%)	183 (88%)	22 (11%)	3 (1%)	11	10
1	I	210/227 (92%)	196 (93%)	11 (5%)	3 (1%)	11	10
1	J	211/227 (93%)	194 (92%)	15 (7%)	2 (1%)	17	20
All	All	2094/2270 (92%)	1939 (93%)	123 (6%)	32 (2%)	10	9

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	18	PRO
1	F	3	GLN
1	F	134	SER
1	F	166	SER
1	G	150	SER
1	H	147	TRP
1	H	194	PRO
1	I	18	PRO
1	A	-3	ASP
1	C	190	CYS
1	F	17	SER
1	F	64	SER
1	F	135	GLU
1	G	64	SER
1	G	132	VAL
1	G	206	GLU
1	I	16	ARG
1	D	19	MET
1	F	173	LYS
1	I	15	ASN
1	J	17	SER
1	A	18	PRO
1	F	4	ALA
1	F	111	HIS

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Mol	Chain	Res	Type
1	G	163	VAL
1	G	168	TYR
1	C	20	TYR
1	G	134	SER
1	J	16	ARG
1	A	17	SER
1	G	137	GLY
1	H	34	GLY

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	A	194/205 (95%)	184 (95%)	10 (5%)	23	31
1	B	192/205 (94%)	180 (94%)	12 (6%)	18	23
1	C	199/205 (97%)	183 (92%)	16 (8%)	12	14
1	D	197/205 (96%)	182 (92%)	15 (8%)	13	16
1	E	192/205 (94%)	183 (95%)	9 (5%)	26	35
1	F	188/205 (92%)	173 (92%)	15 (8%)	12	14
1	G	192/205 (94%)	166 (86%)	26 (14%)	4	3
1	H	193/205 (94%)	177 (92%)	16 (8%)	11	12
1	I	193/205 (94%)	174 (90%)	19 (10%)	8	8
1	J	193/205 (94%)	182 (94%)	11 (6%)	20	26
All	All	1933/2050 (94%)	1784 (92%)	149 (8%)	13	15

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	ASP
1	A	-3	ASP
1	A	11	SER
1	A	16	ARG
1	A	57	GLN

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Mol	Chain	Res	Type
1	A	91	THR
1	A	136	GLU
1	A	175	GLU
1	A	189	SER
1	A	207	ARG
1	B	-4	ASP
1	B	-3	ASP
1	B	1	HIS
1	B	15	ASN
1	B	16	ARG
1	B	25	LYS
1	B	45	SER
1	B	74	ASN
1	B	81	SER
1	B	99	VAL
1	B	157	LYS
1	B	207	ARG
1	C	-7	ASP
1	C	15	ASN
1	C	19	MET
1	C	25	LYS
1	C	57	GLN
1	C	66	MET
1	C	74	ASN
1	C	81	SER
1	C	97[A]	ARG
1	C	97[B]	ARG
1	C	157	LYS
1	C	162[A]	GLN
1	C	162[B]	GLN
1	C	193	GLU
1	C	196	ILE
1	C	207	ARG
1	D	-3	ASP
1	D	0	LEU
1	D	11	SER
1	D	16	ARG
1	D	20	TYR
1	D	46	SER
1	D	76	THR
1	D	80	THR
1	D	99	VAL

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Mol	Chain	Res	Type
1	D	160	THR
1	D	167	SER
1	D	189	SER
1	D	207[A]	ARG
1	D	207[B]	ARG
1	D	208	ARG
1	E	-2	ASP
1	E	0	LEU
1	E	24	THR
1	E	25	LYS
1	E	42	LYS
1	E	135	GLU
1	E	193	GLU
1	E	207	ARG
1	E	208	ARG
1	F	1	HIS
1	F	15	ASN
1	F	26	ASP
1	F	33	LEU
1	F	57	GLN
1	F	77	ASP
1	F	94	SER
1	F	104	PRO
1	F	135	GLU
1	F	157	LYS
1	F	160	THR
1	F	166	SER
1	F	182	THR
1	F	203	LYS
1	F	207	ARG
1	G	-4	ASP
1	G	2	SER
1	G	15	ASN
1	G	24	THR
1	G	37	LEU
1	G	41	VAL
1	G	45	SER
1	G	46	SER
1	G	59	ARG
1	G	66	MET
1	G	77	ASP
1	G	91	THR

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Mol	Chain	Res	Type
1	G	102	LEU
1	G	105	GLN
1	G	110	THR
1	G	114	SER
1	G	132	VAL
1	G	136	GLU
1	G	156	LEU
1	G	167	SER
1	G	171	SER
1	G	177	LEU
1	G	190	CYS
1	G	191	CYS
1	G	202	VAL
1	G	207	ARG
1	H	16	ARG
1	H	40	ILE
1	H	46	SER
1	H	55	TYR
1	H	57	GLN
1	H	59	ARG
1	H	97	ARG
1	H	124	SER
1	H	135	GLU
1	H	152	PHE
1	H	156	LEU
1	H	160	THR
1	H	167	SER
1	H	193	GLU
1	H	205	ARG
1	H	208	ARG
1	I	-3	ASP
1	I	0	LEU
1	I	15	ASN
1	I	16	ARG
1	I	18	PRO
1	I	57	GLN
1	I	80	THR
1	I	91	THR
1	I	94	SER
1	I	95	SER
1	I	105	GLN
1	I	133	ASP

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Mol	Chain	Res	Type
1	I	161	ASP
1	I	180	THR
1	I	182	THR
1	I	193	GLU
1	I	197	ASP
1	I	203	LYS
1	I	205	ARG
1	J	-5	LYS
1	J	-1	LYS
1	J	0	LEU
1	J	15	ASN
1	J	19	MET
1	J	59	ARG
1	J	97	ARG
1	J	105	GLN
1	J	135	GLU
1	J	160	THR
1	J	171	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	105	GLN
1	B	15	ASN
1	B	105	GLN
1	C	15	ASN
1	C	74	ASN
1	C	105	GLN
1	C	186	GLN
1	D	1	HIS
1	D	187	HIS
1	E	63	ASN
1	E	184	GLN
1	F	3	GLN
1	F	38	GLN
1	F	105	GLN
1	F	184	GLN
1	G	15	ASN
1	G	57	GLN
1	G	105	GLN
1	H	57	GLN

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Mol	Chain	Res	Type
1	H	105	GLN
1	H	184	GLN
1	H	187	HIS
1	H	199	ASN
1	I	105	GLN
1	I	184	GLN
1	J	63	ASN
1	J	74	ASN
1	J	105	GLN
1	J	184	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 16 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
3	TUB	E	220	-	50,51,51	1.78	8 (16%)	73,77,77	4.37	22 (30%)

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
3	TUB	E	220	-	-	5/20/49/49	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	220	TUB	O21-C22	6.79	1.54	1.39
3	E	220	TUB	O37-C1	4.73	1.44	1.37
3	E	220	TUB	C12-C11	3.59	1.45	1.40
3	E	220	TUB	O38-C29	3.43	1.43	1.36
3	E	220	TUB	O21-C2	3.31	1.46	1.39
3	E	220	TUB	C4-C7	-3.01	1.47	1.52
3	E	220	TUB	C5-C4	3.01	1.44	1.40
3	E	220	TUB	C11-C16	-2.16	1.36	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	220	TUB	O21-C22-C29	19.58	152.85	116.22
3	E	220	TUB	C35-C26-C25	-15.70	93.50	120.44
3	E	220	TUB	O21-C22-C25	-13.64	81.68	121.80
3	E	220	TUB	C35-C26-C27	12.76	146.23	120.91
3	E	220	TUB	C22-O21-C2	8.55	138.40	118.04
3	E	220	TUB	C5-C4-C7	7.14	129.81	121.57
3	E	220	TUB	O37-C1-C2	6.39	124.31	115.41
3	E	220	TUB	C39-O34-C16	6.06	128.22	118.48
3	E	220	TUB	C9-C10-C5	-5.32	101.88	111.35
3	E	220	TUB	C3-C4-C7	-5.18	111.61	119.39
3	E	220	TUB	C35-C20-N19	4.95	123.20	112.39
3	E	220	TUB	O37-C1-C6	-4.21	116.87	124.12
3	E	220	TUB	C23-C7-N8	-4.06	101.02	111.17
3	E	220	TUB	C10-C5-C4	-3.35	116.11	121.13
3	E	220	TUB	C23-C7-C4	-3.09	106.33	111.66
3	E	220	TUB	C30-C31-C39	-2.68	116.45	119.73
3	E	220	TUB	C18-N19-C20	-2.48	103.71	109.61
3	E	220	TUB	C10-C9-N8	2.28	115.60	111.75
3	E	220	TUB	O21-C2-C1	2.24	123.90	116.87
3	E	220	TUB	O21-C2-C3	-2.19	115.35	121.80
3	E	220	TUB	O34-C16-C15	2.18	124.09	116.88
3	E	220	TUB	C32-C39-C31	2.04	123.32	120.18

There are no chirality outliers.

All (5) torsion outliers are listed below:

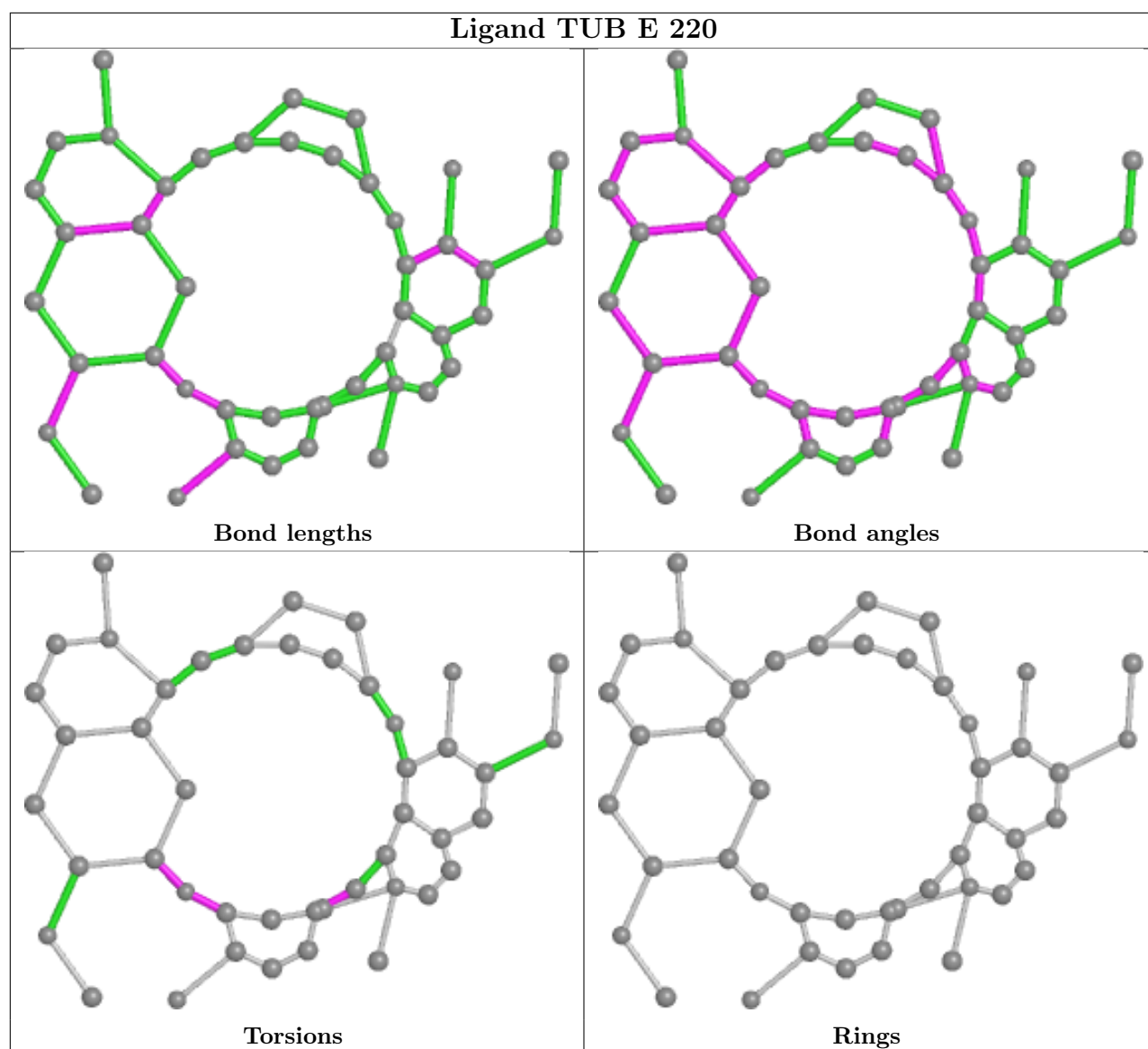
Mol	Chain	Res	Type	Atoms
3	E	220	TUB	C29-C22-O21-C2
3	E	220	TUB	C27-C26-C35-C20
3	E	220	TUB	C25-C26-C35-C20
3	E	220	TUB	C25-C22-O21-C2
3	E	220	TUB	C1-C2-O21-C22

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	220	TUB	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	213/227 (93%)	-0.18	6 (2%)	53	49	17, 31, 56, 71	0
1	B	211/227 (92%)	-0.14	5 (2%)	59	54	19, 33, 61, 72	0
1	C	215/227 (94%)	-0.20	6 (2%)	53	49	17, 30, 61, 84	0
1	D	214/227 (94%)	-0.13	4 (1%)	66	63	14, 25, 60, 73	0
1	E	211/227 (92%)	-0.28	1 (0%)	91	91	13, 25, 49, 76	0
1	F	207/227 (91%)	0.30	14 (6%)	17	13	31, 49, 66, 74	0
1	G	211/227 (92%)	0.59	15 (7%)	16	12	32, 57, 79, 84	0
1	H	212/227 (93%)	0.42	14 (6%)	18	14	30, 56, 77, 87	0
1	I	212/227 (93%)	-0.12	2 (0%)	84	83	23, 40, 64, 77	0
1	J	213/227 (93%)	-0.16	6 (2%)	53	49	22, 36, 61, 79	0
All	All	2119/2270 (93%)	0.01	73 (3%)	45	42	13, 37, 69, 87	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	191	CYS	5.3
1	H	19	MET	5.1
1	G	137	GLY	5.0
1	B	189	SER	4.8
1	C	-6	TYR	4.4
1	G	189	SER	4.2
1	C	190	CYS	4.2
1	G	37	LEU	3.9
1	H	208	ARG	3.6
1	I	18	PRO	3.6
1	H	194	PRO	3.6
1	F	70	ASN	3.5
1	B	190	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	190	CYS	3.4
1	J	18	PRO	3.2
1	F	18	PRO	3.2
1	E	-3	ASP	3.2
1	F	1	HIS	3.1
1	H	177	LEU	3.1
1	I	19	MET	3.0
1	G	152	PHE	3.0
1	G	174	TYR	3.0
1	F	136	GLU	2.9
1	B	188	TYR	2.9
1	G	70	ASN	2.9
1	A	70	ASN	2.8
1	G	25	LYS	2.8
1	A	0	LEU	2.7
1	A	1	HIS	2.7
1	C	191	CYS	2.7
1	F	177	LEU	2.6
1	D	189	SER	2.6
1	C	19	MET	2.6
1	F	202	VAL	2.6
1	B	1	HIS	2.6
1	G	136	GLU	2.6
1	F	133	ASP	2.5
1	C	189	SER	2.5
1	D	-2	ASP	2.5
1	J	-4	ASP	2.4
1	G	133	ASP	2.4
1	H	-2	ASP	2.4
1	J	1	HIS	2.4
1	J	73	GLY	2.4
1	F	139	THR	2.4
1	C	188	TYR	2.3
1	F	4	ALA	2.3
1	F	174	TYR	2.3
1	A	18	PRO	2.2
1	H	134	SER	2.2
1	F	43	ALA	2.2
1	D	16	ARG	2.2
1	H	-3	ASP	2.2
1	J	74	ASN	2.2
1	H	132	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	205	ARG	2.2
1	F	138	ALA	2.2
1	H	190	CYS	2.2
1	G	-5	LYS	2.1
1	G	188	TYR	2.1
1	H	185	VAL	2.1
1	B	-3	ASP	2.1
1	D	0	LEU	2.1
1	H	136	GLU	2.1
1	A	-2	ASP	2.1
1	F	137	GLY	2.1
1	G	-3	ASP	2.0
1	H	137	GLY	2.0
1	A	208	ARG	2.0
1	H	63	ASN	2.0
1	H	152	PHE	2.0
1	F	68	ASP	2.0
1	J	136	GLU	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 monosaccharides in this entry.

6.4 Ligands [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. 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	B-factors(Å ²)	Q<0.9
2	MG	C	220	1/1	0.40	0.25	40,40,40,40	0
2	MG	I	221	1/1	0.40	0.39	52,52,52,52	0
2	MG	E	222	1/1	0.42	0.58	36,36,36,36	0
2	MG	B	221	1/1	0.48	0.28	53,53,53,53	0
2	MG	A	221	1/1	0.61	0.30	43,43,43,43	0

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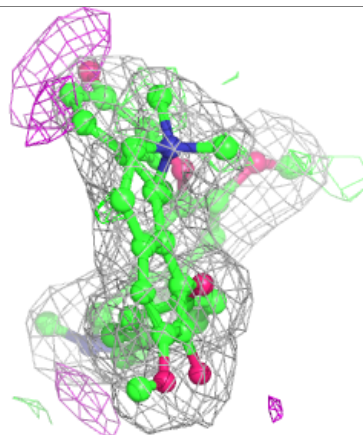
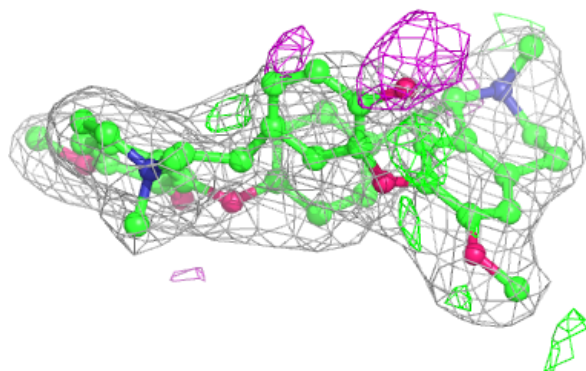
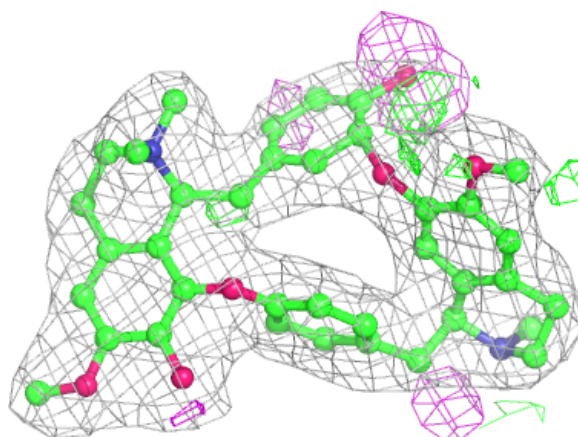
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	E	221	1/1	0.68	0.33	45,45,45,45	0
2	MG	D	222	1/1	0.73	0.24	48,48,48,48	0
2	MG	B	220	1/1	0.74	0.28	44,44,44,44	0
2	MG	D	220	1/1	0.76	0.15	49,49,49,49	0
2	MG	J	220	1/1	0.76	0.33	46,46,46,46	0
2	MG	G	220	1/1	0.82	0.16	55,55,55,55	0
2	MG	F	220	1/1	0.89	0.20	54,54,54,54	0
2	MG	F	221	1/1	0.90	0.29	52,52,52,52	0
3	TUB	E	220	45/45	0.93	0.20	15,20,26,28	0
2	MG	D	221	1/1	0.95	0.15	57,57,57,57	0
2	MG	A	220	1/1	0.97	0.27	43,43,43,43	0
2	MG	I	220	1/1	0.98	0.30	43,43,43,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TUB E 220:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.