wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 12:15 pm GMT

PDB ID	:	1UW6
Title	:	X-ray structure of acetylcholine binding protein (AChBP) in complex with nicotine
Authors	:	Celie, P.H.N.; Van Rossum-fikkert, S.E.; Van Dijk, W.J.; Brejc, K.; Smit, A.B.; Sixma, T.K.
Deposited on	:	2004-01-30
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

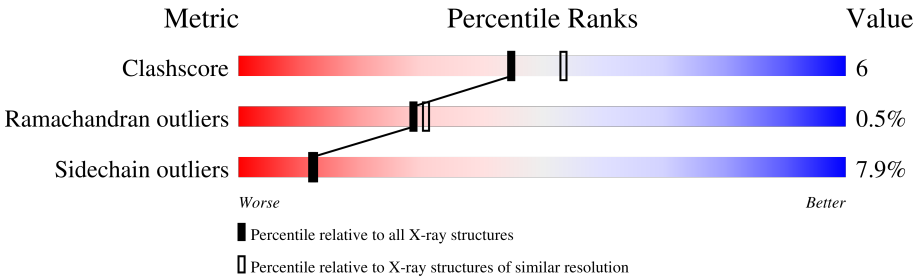
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	211	81% 15%
1	B	211	78% 17%
1	C	211	81% 12%
1	D	211	80% 15%
1	E	211	81% 16%
1	F	211	84% 11%
1	G	211	85% 11%
1	H	211	78% 18%

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Mol	Chain	Length	Quality of chain
1	I	211	
1	J	211	
1	K	211	
1	L	211	
1	M	211	
1	N	211	
1	O	211	
1	P	211	
1	Q	211	
1	R	211	
1	S	211	
1	T	211	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 34788 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 ACETYLCHOLINE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1665	1040	286	334	5			
1	B	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	C	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	D	208	Total	C	N	O	S	0	0	0
			1665	1040	286	334	5			
1	E	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	F	208	Total	C	N	O	S	0	0	0
			1665	1040	286	334	5			
1	G	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	H	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	I	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	J	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	K	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	L	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	M	208	Total	C	N	O	S	0	0	0
			1665	1040	286	334	5			
1	N	208	Total	C	N	O	S	0	0	0
			1665	1040	286	334	5			
1	O	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	P	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	R	208	Total	C	N	O	S	0	0	0
			1665	1040	286	334	5			
1	S	206	Total	C	N	O	S	0	0	0
			1648	1031	281	331	5			
1	T	208	Total	C	N	O	S	0	0	0
			1665	1040	286	334	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLU	SER	conflict	UNP P58154
A	1	PHE	LEU	conflict	UNP P58154
B	0	GLU	SER	conflict	UNP P58154
B	1	PHE	LEU	conflict	UNP P58154
C	0	GLU	SER	conflict	UNP P58154
C	1	PHE	LEU	conflict	UNP P58154
D	0	GLU	SER	conflict	UNP P58154
D	1	PHE	LEU	conflict	UNP P58154
E	0	GLU	SER	conflict	UNP P58154
E	1	PHE	LEU	conflict	UNP P58154
F	0	GLU	SER	conflict	UNP P58154
F	1	PHE	LEU	conflict	UNP P58154
G	0	GLU	SER	conflict	UNP P58154
G	1	PHE	LEU	conflict	UNP P58154
H	0	GLU	SER	conflict	UNP P58154
H	1	PHE	LEU	conflict	UNP P58154
I	0	GLU	SER	conflict	UNP P58154
I	1	PHE	LEU	conflict	UNP P58154
J	0	GLU	SER	conflict	UNP P58154
J	1	PHE	LEU	conflict	UNP P58154
K	0	GLU	SER	conflict	UNP P58154
K	1	PHE	LEU	conflict	UNP P58154
L	0	GLU	SER	conflict	UNP P58154
L	1	PHE	LEU	conflict	UNP P58154
M	0	GLU	SER	conflict	UNP P58154
M	1	PHE	LEU	conflict	UNP P58154
N	0	GLU	SER	conflict	UNP P58154
N	1	PHE	LEU	conflict	UNP P58154
O	0	GLU	SER	conflict	UNP P58154
O	1	PHE	LEU	conflict	UNP P58154
P	0	GLU	SER	conflict	UNP P58154

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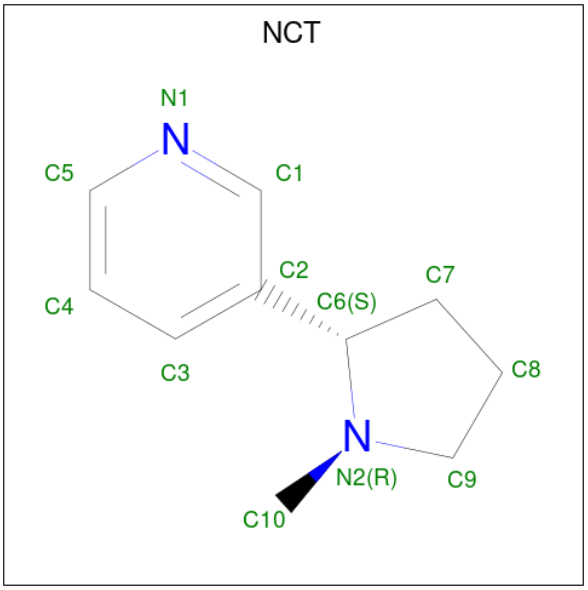
Chain	Residue	Modelled	Actual	Comment	Reference
P	1	PHE	LEU	conflict	UNP P58154
Q	0	GLU	SER	conflict	UNP P58154
Q	1	PHE	LEU	conflict	UNP P58154
R	0	GLU	SER	conflict	UNP P58154
R	1	PHE	LEU	conflict	UNP P58154
S	0	GLU	SER	conflict	UNP P58154
S	1	PHE	LEU	conflict	UNP P58154
T	0	GLU	SER	conflict	UNP P58154
T	1	PHE	LEU	conflict	UNP P58154

- Molecule 2 is (S)-3-(1-METHYLPYRROLIDIN-2-YL)PYRIDINE (three-letter code: NCT) (formula: $C_{10}H_{14}N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 12 10 2	0	0
2	B	1	Total C N 12 10 2	0	0
2	C	1	Total C N 12 10 2	0	0
2	D	1	Total C N 12 10 2	0	0
2	E	1	Total C N 12 10 2	0	0
2	F	1	Total C N 12 10 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C N 12 10 2	0	0
2	H	1	Total C N 12 10 2	0	0
2	I	1	Total C N 12 10 2	0	0
2	J	1	Total C N 12 10 2	0	0
2	K	1	Total C N 12 10 2	0	0
2	L	1	Total C N 12 10 2	0	0
2	M	1	Total C N 12 10 2	0	0
2	N	1	Total C N 12 10 2	0	0
2	O	1	Total C N 12 10 2	0	0
2	P	1	Total C N 12 10 2	0	0
2	Q	1	Total C N 12 10 2	0	0
2	R	1	Total C N 12 10 2	0	0
2	S	1	Total C N 12 10 2	0	0
2	T	1	Total C N 12 10 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	90	Total O 90 90	0	0
3	B	85	Total O 85 85	0	0
3	C	81	Total O 81 81	0	0
3	D	73	Total O 73 73	0	0
3	E	63	Total O 63 63	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	84	Total O 84 84	0	0
3	G	62	Total O 62 62	0	0
3	H	60	Total O 60 60	0	0
3	I	71	Total O 71 71	0	0
3	J	70	Total O 70 70	0	0
3	K	55	Total O 55 55	0	0
3	L	41	Total O 41 41	0	0
3	M	81	Total O 81 81	0	0
3	N	80	Total O 80 80	0	0
3	O	71	Total O 71 71	0	0
3	P	95	Total O 95 95	0	0
3	Q	75	Total O 75 75	0	0
3	R	74	Total O 74 74	0	0
3	S	68	Total O 68 68	0	0
3	T	90	Total O 90 90	0	0

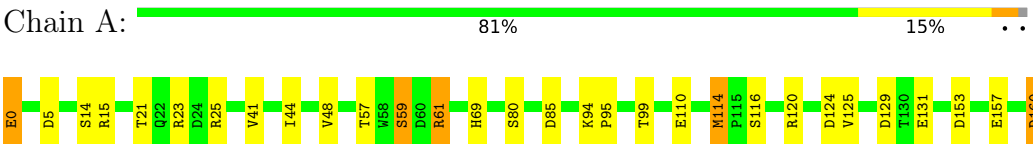
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

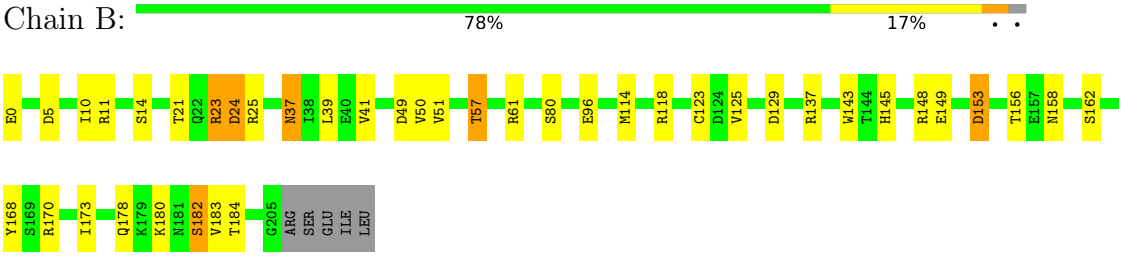
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain A:



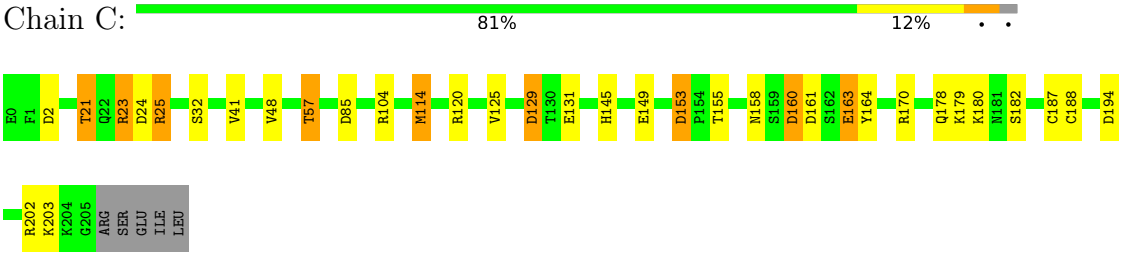
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain B:



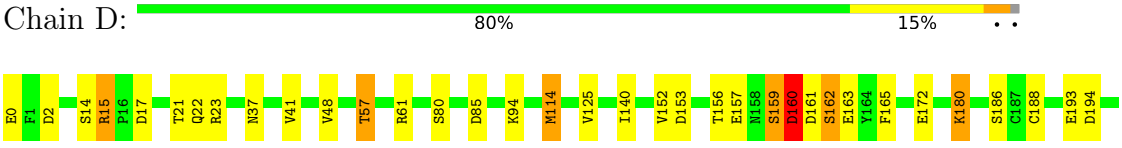
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

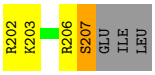
Chain C:



• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

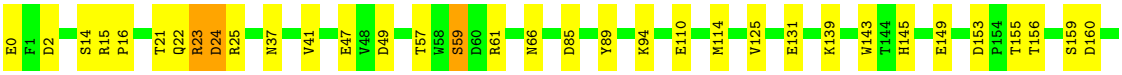
Chain D:

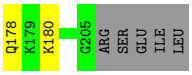




• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

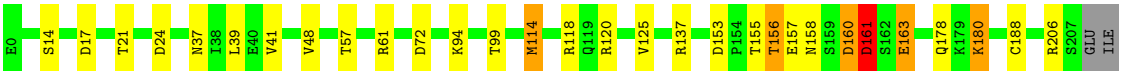
Chain E:





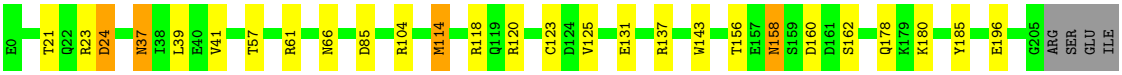
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain F:



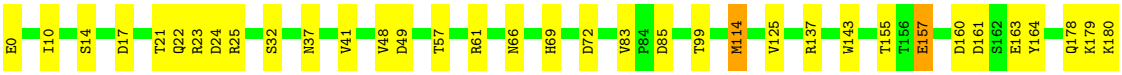
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

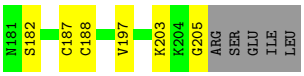
Chain G:



• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

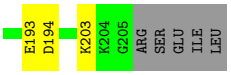
Chain H:





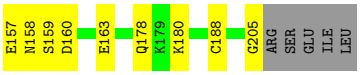
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain I:



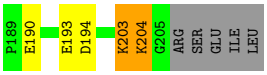
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain J:



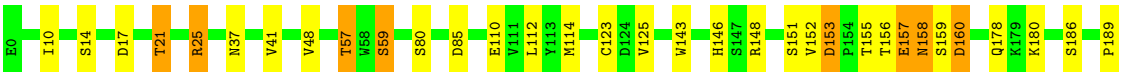
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

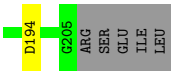
Chain K:



• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain L:



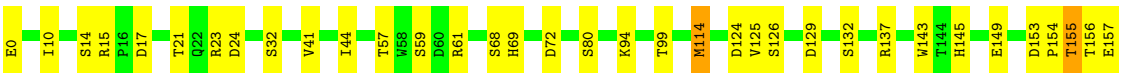


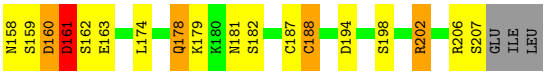
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain M:

• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

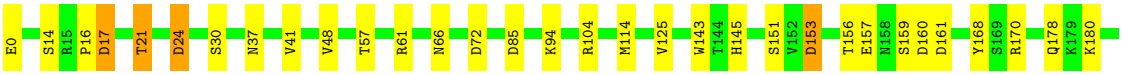
Chain N:





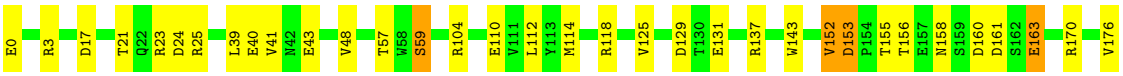
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

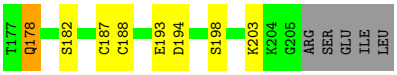
Chain O:



• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

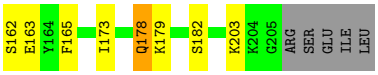
Chain P:





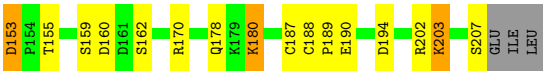
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain Q:



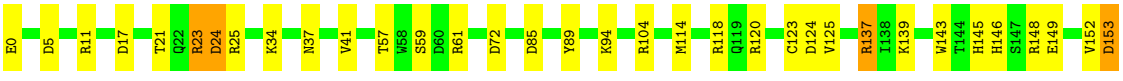
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

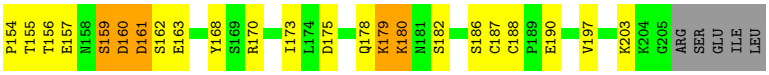
Chain R:



• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

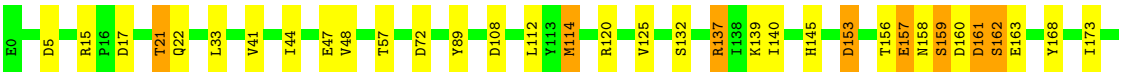
Chain S:

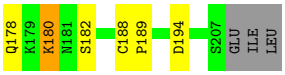




• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain T:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	233.00Å 267.42Å 73.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.20	Depositor
% Data completeness (in resolution range)	84.2 (12.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.222 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	34788	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.73	0/1702	0.89	5/2321 (0.2%)
1	B	0.78	0/1685	0.90	5/2299 (0.2%)
1	C	0.78	0/1685	0.88	7/2299 (0.3%)
1	D	0.79	1/1702 (0.1%)	0.87	7/2321 (0.3%)
1	E	0.68	0/1685	0.84	5/2299 (0.2%)
1	F	0.72	0/1702	0.86	4/2321 (0.2%)
1	G	0.70	0/1685	0.85	4/2299 (0.2%)
1	H	1.76	1/1685 (0.1%)	1.28	6/2299 (0.3%)
1	I	0.72	0/1685	0.89	6/2299 (0.3%)
1	J	0.76	1/1685 (0.1%)	0.94	4/2299 (0.2%)
1	K	0.69	0/1685	0.84	5/2299 (0.2%)
1	L	0.61	0/1685	0.84	4/2299 (0.2%)
1	M	0.70	0/1702	0.89	7/2321 (0.3%)
1	N	0.73	0/1702	0.89	7/2321 (0.3%)
1	O	0.97	1/1685 (0.1%)	0.88	7/2299 (0.3%)
1	P	0.77	0/1685	0.87	4/2299 (0.2%)
1	Q	0.76	0/1685	0.89	3/2299 (0.1%)
1	R	0.76	0/1702	0.91	8/2321 (0.3%)
1	S	0.73	0/1685	0.89	9/2299 (0.4%)
1	T	0.76	0/1702	0.90	6/2321 (0.3%)
All	All	0.83	4/33819 (0.0%)	0.90	113/46134 (0.2%)

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	B	0	1
1	F	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	205	GLY	C-O	66.80	2.30	1.23
1	O	205	GLY	C-O	25.32	1.64	1.23
1	D	207	SER	C-O	-15.66	0.93	1.23
1	J	205	GLY	C-O	5.75	1.32	1.23

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	205	GLY	CA-C-O	-45.27	39.12	120.60
1	J	205	GLY	CA-C-O	-18.43	87.43	120.60
1	I	129	ASP	CB-CG-OD2	9.40	126.76	118.30
1	M	17	ASP	CB-CG-OD2	7.82	125.34	118.30
1	R	153	ASP	CB-CG-OD2	7.71	125.24	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	158	ASN	Peptide
1	F	160	ASP	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	1665	0	1603	24	0
1	B	1648	0	1585	28	0
1	C	1648	0	1585	19	0
1	D	1665	0	1603	18	0
1	E	1648	0	1585	14	0
1	F	1665	0	1603	15	0
1	G	1648	0	1585	13	0
1	H	1648	0	1585	26	0
1	I	1648	0	1585	20	0
1	J	1648	0	1585	31	0
1	K	1648	0	1585	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1648	0	1585	19	0
1	M	1665	0	1603	23	0
1	N	1665	0	1603	29	0
1	O	1648	0	1585	18	0
1	P	1648	0	1585	27	0
1	Q	1648	0	1585	33	0
1	R	1665	0	1603	32	0
1	S	1648	0	1585	44	0
1	T	1665	0	1603	22	0
2	A	12	0	14	0	0
2	B	12	0	14	1	0
2	C	12	0	14	0	0
2	D	12	0	14	0	0
2	E	12	0	14	1	0
2	F	12	0	14	0	0
2	G	12	0	14	0	0
2	H	12	0	14	3	0
2	I	12	0	14	0	0
2	J	12	0	14	0	0
2	K	12	0	14	0	0
2	L	12	0	14	0	0
2	M	12	0	14	0	0
2	N	12	0	14	1	0
2	O	12	0	14	1	0
2	P	12	0	14	0	0
2	Q	12	0	14	1	0
2	R	12	0	14	0	0
2	S	12	0	14	1	0
2	T	12	0	14	0	0
3	A	90	0	0	4	0
3	B	85	0	0	8	0
3	C	81	0	0	7	0
3	D	73	0	0	6	0
3	E	63	0	0	2	0
3	F	84	0	0	4	0
3	G	62	0	0	4	0
3	H	60	0	0	6	3
3	I	71	0	0	8	0
3	J	70	0	0	1	0
3	K	55	0	0	6	0
3	L	41	0	0	5	0
3	M	81	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	80	0	0	7	0
3	O	71	0	0	7	0
3	P	95	0	0	8	0
3	Q	75	0	0	9	0
3	R	74	0	0	9	1
3	S	68	0	0	4	0
3	T	90	0	0	4	0
All	All	34788	0	32106	424	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 6.

The worst 5 of 424 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:O:205:GLY:O	1:O:205:GLY:C	1.64	1.35
1:B:23:ARG:HG3	1:B:23:ARG:HH11	1.27	1.00
1:P:3:ARG:NH1	3:P:2002:HOH:O	2.01	0.93
1:H:137:ARG:HD2	3:H:2040:HOH:O	1.71	0.90
1:S:137:ARG:HD2	3:S:2050:HOH:O	1.73	0.89

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)
3:H:2060:HOH:O	3:H:2060:HOH:O[2_665]	1.45	0.75
3:H:2036:HOH:O	3:H:2036:HOH:O[2_665]	1.76	0.44
3:H:2018:HOH:O	3:R:2023:HOH:O[3_546]	2.10	0.10

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	206/211 (98%)	205 (100%)	1 (0%)	0	100	100
1	B	204/211 (97%)	201 (98%)	3 (2%)	0	100	100
1	C	204/211 (97%)	199 (98%)	4 (2%)	1 (0%)	29	31
1	D	206/211 (98%)	198 (96%)	6 (3%)	2 (1%)	15	14
1	E	204/211 (97%)	197 (97%)	6 (3%)	1 (0%)	29	31
1	F	206/211 (98%)	198 (96%)	8 (4%)	0	100	100
1	G	204/211 (97%)	199 (98%)	5 (2%)	0	100	100
1	H	204/211 (97%)	202 (99%)	2 (1%)	0	100	100
1	I	204/211 (97%)	197 (97%)	5 (2%)	2 (1%)	15	14
1	J	204/211 (97%)	198 (97%)	5 (2%)	1 (0%)	29	31
1	K	204/211 (97%)	201 (98%)	2 (1%)	1 (0%)	29	31
1	L	204/211 (97%)	200 (98%)	3 (2%)	1 (0%)	29	31
1	M	206/211 (98%)	204 (99%)	2 (1%)	0	100	100
1	N	206/211 (98%)	201 (98%)	2 (1%)	3 (2%)	10	8
1	O	204/211 (97%)	196 (96%)	8 (4%)	0	100	100
1	P	204/211 (97%)	197 (97%)	7 (3%)	0	100	100
1	Q	204/211 (97%)	197 (97%)	4 (2%)	3 (2%)	10	8
1	R	206/211 (98%)	202 (98%)	3 (2%)	1 (0%)	29	31
1	S	204/211 (97%)	197 (97%)	5 (2%)	2 (1%)	15	14
1	T	206/211 (98%)	203 (98%)	1 (0%)	2 (1%)	15	14
All	All	4094/4220 (97%)	3992 (98%)	82 (2%)	20 (0%)	29	31

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	159	SER
1	D	160	ASP
1	I	23	ARG
1	Q	161	ASP
1	S	23	ARG

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	194/197 (98%)	180 (93%)	14 (7%)	14	15
1	B	192/197 (98%)	179 (93%)	13 (7%)	16	17
1	C	192/197 (98%)	178 (93%)	14 (7%)	14	15
1	D	194/197 (98%)	176 (91%)	18 (9%)	9	8
1	E	192/197 (98%)	175 (91%)	17 (9%)	9	9
1	F	194/197 (98%)	176 (91%)	18 (9%)	9	8
1	G	192/197 (98%)	179 (93%)	13 (7%)	16	17
1	H	192/197 (98%)	181 (94%)	11 (6%)	20	24
1	I	192/197 (98%)	174 (91%)	18 (9%)	8	8
1	J	192/197 (98%)	179 (93%)	13 (7%)	16	17
1	K	192/197 (98%)	177 (92%)	15 (8%)	12	13
1	L	192/197 (98%)	178 (93%)	14 (7%)	14	15
1	M	194/197 (98%)	176 (91%)	18 (9%)	9	8
1	N	194/197 (98%)	174 (90%)	20 (10%)	7	6
1	O	192/197 (98%)	180 (94%)	12 (6%)	18	20
1	P	192/197 (98%)	177 (92%)	15 (8%)	12	13
1	Q	192/197 (98%)	176 (92%)	16 (8%)	11	11
1	R	194/197 (98%)	180 (93%)	14 (7%)	14	15
1	S	192/197 (98%)	174 (91%)	18 (9%)	8	8
1	T	194/197 (98%)	181 (93%)	13 (7%)	16	18
All	All	3854/3940 (98%)	3550 (92%)	304 (8%)	12	12

5 of 304 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	24	ASP
1	S	161	ASP
1	P	155	THR
1	R	21	THR
1	T	159	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	12	GLN
1	Q	146	HIS
1	Q	145	HIS
1	R	145	HIS
1	H	178	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NCT	I	1206	-	13,13,13	0.86	0	17,17,17	1.30	3 (17%)
2	NCT	A	1208	-	13,13,13	1.12	0	17,17,17	1.20	1 (5%)
2	NCT	E	1206	-	13,13,13	0.75	0	17,17,17	1.17	1 (5%)
2	NCT	M	1208	-	13,13,13	0.92	1 (7%)	17,17,17	1.67	3 (17%)
2	NCT	Q	1206	-	13,13,13	0.95	1 (7%)	17,17,17	1.23	3 (17%)
2	NCT	J	1206	-	13,13,13	0.80	0	17,17,17	1.36	5 (29%)
2	NCT	L	1206	-	13,13,13	0.71	0	17,17,17	1.59	3 (17%)
2	NCT	R	1208	-	13,13,13	0.73	0	17,17,17	1.25	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NCT	K	1206	-	13,13,13	0.99	1 (7%)	17,17,17	1.49	3 (17%)
2	NCT	G	1206	-	13,13,13	0.85	0	17,17,17	1.57	4 (23%)
2	NCT	S	1206	-	13,13,13	1.21	2 (15%)	17,17,17	1.54	5 (29%)
2	NCT	F	1208	-	13,13,13	0.84	0	17,17,17	1.48	4 (23%)
2	NCT	B	1206	-	13,13,13	0.97	0	17,17,17	1.14	1 (5%)
2	NCT	T	1208	-	13,13,13	0.74	0	17,17,17	1.09	1 (5%)
2	NCT	O	1206	-	13,13,13	1.19	2 (15%)	17,17,17	1.54	4 (23%)
2	NCT	C	1206	-	13,13,13	1.03	1 (7%)	17,17,17	1.31	2 (11%)
2	NCT	D	1208	-	13,13,13	0.74	0	17,17,17	1.45	3 (17%)
2	NCT	H	1206	-	13,13,13	0.75	0	17,17,17	1.59	5 (29%)
2	NCT	P	1206	-	13,13,13	0.89	1 (7%)	17,17,17	1.59	4 (23%)
2	NCT	N	1208	-	13,13,13	0.88	1 (7%)	17,17,17	1.21	1 (5%)

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
2	NCT	I	1206	-	-	1/4/14/14	0/2/2/2
2	NCT	A	1208	-	-	1/4/14/14	0/2/2/2
2	NCT	E	1206	-	-	0/4/14/14	0/2/2/2
2	NCT	M	1208	-	-	0/4/14/14	0/2/2/2
2	NCT	Q	1206	-	-	3/4/14/14	0/2/2/2
2	NCT	J	1206	-	-	2/4/14/14	0/2/2/2
2	NCT	L	1206	-	-	2/4/14/14	0/2/2/2
2	NCT	R	1208	-	-	1/4/14/14	0/2/2/2
2	NCT	K	1206	-	-	0/4/14/14	0/2/2/2
2	NCT	G	1206	-	-	1/4/14/14	0/2/2/2
2	NCT	S	1206	-	-	4/4/14/14	0/2/2/2
2	NCT	F	1208	-	-	1/4/14/14	0/2/2/2
2	NCT	B	1206	-	-	4/4/14/14	0/2/2/2
2	NCT	T	1208	-	-	0/4/14/14	0/2/2/2
2	NCT	O	1206	-	-	1/4/14/14	0/2/2/2
2	NCT	C	1206	-	-	1/4/14/14	0/2/2/2
2	NCT	D	1208	-	-	1/4/14/14	0/2/2/2
2	NCT	H	1206	-	-	1/4/14/14	0/2/2/2
2	NCT	P	1206	-	-	1/4/14/14	0/2/2/2
2	NCT	N	1208	-	-	1/4/14/14	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1206	NCT	C2-C6	-3.23	1.47	1.51
2	S	1206	NCT	C2-C6	-2.90	1.47	1.51
2	Q	1206	NCT	C2-C6	-2.67	1.47	1.51
2	M	1208	NCT	C2-C6	-2.56	1.48	1.51
2	K	1206	NCT	C2-C6	-2.48	1.48	1.51

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	1208	NCT	C5-N1-C1	3.88	123.56	116.85
2	G	1206	NCT	C5-N1-C1	3.87	123.54	116.85
2	M	1208	NCT	C2-C1-N1	-3.70	118.33	124.14
2	L	1206	NCT	C5-N1-C1	3.41	122.75	116.85
2	P	1206	NCT	C5-N1-C1	3.32	122.60	116.85

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1206	NCT	C1-C2-C6-N2
2	Q	1206	NCT	C1-C2-C6-N2
2	S	1206	NCT	C1-C2-C6-N2
2	B	1206	NCT	C3-C2-C6-N2
2	S	1206	NCT	C3-C2-C6-N2

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1206	NCT	1	0
2	Q	1206	NCT	1	0
2	S	1206	NCT	1	0
2	B	1206	NCT	1	0
2	O	1206	NCT	1	0
2	H	1206	NCT	3	0
2	N	1208	NCT	1	0

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.