



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:40 AM UTC

PDB ID : 3T4M / pdb_00003t4m
Title : Ac-AChBP ligand binding domain mutated to human alpha-7 nAChR (inter-mediate)
Authors : Nemecz, A.; Taylor, P.W.
Deposited on : 2011-07-26
Resolution : 3.00 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

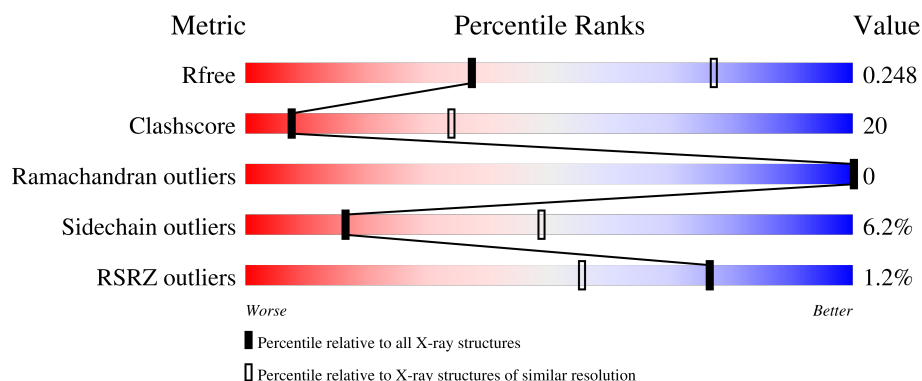
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	230	
1	B	230	
1	C	230	
1	D	230	
1	E	230	

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Mol	Chain	Length	Quality of chain
1	F	230	% 60% 29% • 7%
1	G	230	2% 52% 36% 6% 7%
1	H	230	2% 52% 37% 5% 7%
1	I	230	2% 50% 37% 6% 7%
1	J	230	57% 33% • 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17570 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	214	Total	C	N	O	S	0	2	0
			1733	1090	289	346	8			
1	B	214	Total	C	N	O	S	0	1	0
			1722	1083	283	348	8			
1	C	214	Total	C	N	O	S	0	1	0
			1724	1084	288	344	8			
1	D	215	Total	C	N	O	S	0	2	0
			1739	1093	290	348	8			
1	E	214	Total	C	N	O	S	0	2	0
			1731	1089	287	347	8			
1	F	214	Total	C	N	O	S	0	3	0
			1738	1093	290	347	8			
1	G	215	Total	C	N	O	S	0	1	0
			1737	1094	287	348	8			
1	H	215	Total	C	N	O	S	0	3	0
			1744	1096	291	349	8			
1	I	215	Total	C	N	O	S	0	4	0
			1753	1102	295	347	9			
1	J	213	Total	C	N	O	S	0	4	0
			1733	1090	285	350	8			

There are 230 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP Q8WSF8
A	-7	TYR	-	expression tag	UNP Q8WSF8
A	-6	LYS	-	expression tag	UNP Q8WSF8
A	-5	ASP	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	55	TRP	TYR	engineered mutation	UNP Q8WSF8
A	106	ASN	ILE	engineered mutation	UNP Q8WSF8
A	108	LEU	VAL	engineered mutation	UNP Q8WSF8
A	116	GLN	MET	engineered mutation	UNP Q8WSF8
A	117	TYR	PHE	engineered mutation	UNP Q8WSF8
A	118	LEU	ILE	engineered mutation	UNP Q8WSF8
A	148	SER	VAL	engineered mutation	UNP Q8WSF8
A	186	ARG	GLN	engineered mutation	UNP Q8WSF8
A	187	PHE	HIS	engineered mutation	UNP Q8WSF8
A	189	GLU	SER	engineered mutation	UNP Q8WSF8
A	192	LYS	PRO	engineered mutation	UNP Q8WSF8
A	196	PRO	ILE	engineered mutation	UNP Q8WSF8
A	220	SER	-	expression tag	UNP Q8WSF8
A	221	ARG	-	expression tag	UNP Q8WSF8
B	-8	ASP	-	expression tag	UNP Q8WSF8
B	-7	TYR	-	expression tag	UNP Q8WSF8
B	-6	LYS	-	expression tag	UNP Q8WSF8
B	-5	ASP	-	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
B	55	TRP	TYR	engineered mutation	UNP Q8WSF8
B	106	ASN	ILE	engineered mutation	UNP Q8WSF8
B	108	LEU	VAL	engineered mutation	UNP Q8WSF8
B	116	GLN	MET	engineered mutation	UNP Q8WSF8
B	117	TYR	PHE	engineered mutation	UNP Q8WSF8
B	118	LEU	ILE	engineered mutation	UNP Q8WSF8
B	148	SER	VAL	engineered mutation	UNP Q8WSF8
B	186	ARG	GLN	engineered mutation	UNP Q8WSF8
B	187	PHE	HIS	engineered mutation	UNP Q8WSF8
B	189	GLU	SER	engineered mutation	UNP Q8WSF8
B	192	LYS	PRO	engineered mutation	UNP Q8WSF8
B	196	PRO	ILE	engineered mutation	UNP Q8WSF8
B	220	SER	-	expression tag	UNP Q8WSF8
B	221	ARG	-	expression tag	UNP Q8WSF8
C	-8	ASP	-	expression tag	UNP Q8WSF8
C	-7	TYR	-	expression tag	UNP Q8WSF8
C	-6	LYS	-	expression tag	UNP Q8WSF8
C	-5	ASP	-	expression tag	UNP Q8WSF8
C	-4	ASP	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
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
C	55	TRP	TYR	engineered mutation	UNP Q8WSF8
C	106	ASN	ILE	engineered mutation	UNP Q8WSF8
C	108	LEU	VAL	engineered mutation	UNP Q8WSF8
C	116	GLN	MET	engineered mutation	UNP Q8WSF8
C	117	TYR	PHE	engineered mutation	UNP Q8WSF8
C	118	LEU	ILE	engineered mutation	UNP Q8WSF8
C	148	SER	VAL	engineered mutation	UNP Q8WSF8
C	186	ARG	GLN	engineered mutation	UNP Q8WSF8
C	187	PHE	HIS	engineered mutation	UNP Q8WSF8
C	189	GLU	SER	engineered mutation	UNP Q8WSF8
C	192	LYS	PRO	engineered mutation	UNP Q8WSF8
C	196	PRO	ILE	engineered mutation	UNP Q8WSF8
C	220	SER	-	expression tag	UNP Q8WSF8
C	221	ARG	-	expression tag	UNP Q8WSF8
D	-8	ASP	-	expression tag	UNP Q8WSF8
D	-7	TYR	-	expression tag	UNP Q8WSF8
D	-6	LYS	-	expression tag	UNP Q8WSF8
D	-5	ASP	-	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
D	55	TRP	TYR	engineered mutation	UNP Q8WSF8
D	106	ASN	ILE	engineered mutation	UNP Q8WSF8
D	108	LEU	VAL	engineered mutation	UNP Q8WSF8
D	116	GLN	MET	engineered mutation	UNP Q8WSF8
D	117	TYR	PHE	engineered mutation	UNP Q8WSF8
D	118	LEU	ILE	engineered mutation	UNP Q8WSF8
D	148	SER	VAL	engineered mutation	UNP Q8WSF8
D	186	ARG	GLN	engineered mutation	UNP Q8WSF8
D	187	PHE	HIS	engineered mutation	UNP Q8WSF8
D	189	GLU	SER	engineered mutation	UNP Q8WSF8
D	192	LYS	PRO	engineered mutation	UNP Q8WSF8
D	196	PRO	ILE	engineered mutation	UNP Q8WSF8
D	220	SER	-	expression tag	UNP Q8WSF8
D	221	ARG	-	expression tag	UNP Q8WSF8
E	-8	ASP	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	TYR	-	expression tag	UNP Q8WSF8
E	-6	LYS	-	expression tag	UNP Q8WSF8
E	-5	ASP	-	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
E	55	TRP	TYR	engineered mutation	UNP Q8WSF8
E	106	ASN	ILE	engineered mutation	UNP Q8WSF8
E	108	LEU	VAL	engineered mutation	UNP Q8WSF8
E	116	GLN	MET	engineered mutation	UNP Q8WSF8
E	117	TYR	PHE	engineered mutation	UNP Q8WSF8
E	118	LEU	ILE	engineered mutation	UNP Q8WSF8
E	148	SER	VAL	engineered mutation	UNP Q8WSF8
E	186	ARG	GLN	engineered mutation	UNP Q8WSF8
E	187	PHE	HIS	engineered mutation	UNP Q8WSF8
E	189	GLU	SER	engineered mutation	UNP Q8WSF8
E	192	LYS	PRO	engineered mutation	UNP Q8WSF8
E	196	PRO	ILE	engineered mutation	UNP Q8WSF8
E	220	SER	-	expression tag	UNP Q8WSF8
E	221	ARG	-	expression tag	UNP Q8WSF8
F	-8	ASP	-	expression tag	UNP Q8WSF8
F	-7	TYR	-	expression tag	UNP Q8WSF8
F	-6	LYS	-	expression tag	UNP Q8WSF8
F	-5	ASP	-	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
F	55	TRP	TYR	engineered mutation	UNP Q8WSF8
F	106	ASN	ILE	engineered mutation	UNP Q8WSF8
F	108	LEU	VAL	engineered mutation	UNP Q8WSF8
F	116	GLN	MET	engineered mutation	UNP Q8WSF8
F	117	TYR	PHE	engineered mutation	UNP Q8WSF8
F	118	LEU	ILE	engineered mutation	UNP Q8WSF8
F	148	SER	VAL	engineered mutation	UNP Q8WSF8
F	186	ARG	GLN	engineered mutation	UNP Q8WSF8
F	187	PHE	HIS	engineered mutation	UNP Q8WSF8
F	189	GLU	SER	engineered mutation	UNP Q8WSF8
F	192	LYS	PRO	engineered mutation	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	196	PRO	ILE	engineered mutation	UNP Q8WSF8
F	220	SER	-	expression tag	UNP Q8WSF8
F	221	ARG	-	expression tag	UNP Q8WSF8
G	-8	ASP	-	expression tag	UNP Q8WSF8
G	-7	TYR	-	expression tag	UNP Q8WSF8
G	-6	LYS	-	expression tag	UNP Q8WSF8
G	-5	ASP	-	expression tag	UNP Q8WSF8
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
G	55	TRP	TYR	engineered mutation	UNP Q8WSF8
G	106	ASN	ILE	engineered mutation	UNP Q8WSF8
G	108	LEU	VAL	engineered mutation	UNP Q8WSF8
G	116	GLN	MET	engineered mutation	UNP Q8WSF8
G	117	TYR	PHE	engineered mutation	UNP Q8WSF8
G	118	LEU	ILE	engineered mutation	UNP Q8WSF8
G	148	SER	VAL	engineered mutation	UNP Q8WSF8
G	186	ARG	GLN	engineered mutation	UNP Q8WSF8
G	187	PHE	HIS	engineered mutation	UNP Q8WSF8
G	189	GLU	SER	engineered mutation	UNP Q8WSF8
G	192	LYS	PRO	engineered mutation	UNP Q8WSF8
G	196	PRO	ILE	engineered mutation	UNP Q8WSF8
G	220	SER	-	expression tag	UNP Q8WSF8
G	221	ARG	-	expression tag	UNP Q8WSF8
H	-8	ASP	-	expression tag	UNP Q8WSF8
H	-7	TYR	-	expression tag	UNP Q8WSF8
H	-6	LYS	-	expression tag	UNP Q8WSF8
H	-5	ASP	-	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
H	55	TRP	TYR	engineered mutation	UNP Q8WSF8
H	106	ASN	ILE	engineered mutation	UNP Q8WSF8
H	108	LEU	VAL	engineered mutation	UNP Q8WSF8
H	116	GLN	MET	engineered mutation	UNP Q8WSF8
H	117	TYR	PHE	engineered mutation	UNP Q8WSF8
H	118	LEU	ILE	engineered mutation	UNP Q8WSF8
H	148	SER	VAL	engineered mutation	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	186	ARG	GLN	engineered mutation	UNP Q8WSF8
H	187	PHE	HIS	engineered mutation	UNP Q8WSF8
H	189	GLU	SER	engineered mutation	UNP Q8WSF8
H	192	LYS	PRO	engineered mutation	UNP Q8WSF8
H	196	PRO	ILE	engineered mutation	UNP Q8WSF8
H	220	SER	-	expression tag	UNP Q8WSF8
H	221	ARG	-	expression tag	UNP Q8WSF8
I	-8	ASP	-	expression tag	UNP Q8WSF8
I	-7	TYR	-	expression tag	UNP Q8WSF8
I	-6	LYS	-	expression tag	UNP Q8WSF8
I	-5	ASP	-	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
I	55	TRP	TYR	engineered mutation	UNP Q8WSF8
I	106	ASN	ILE	engineered mutation	UNP Q8WSF8
I	108	LEU	VAL	engineered mutation	UNP Q8WSF8
I	116	GLN	MET	engineered mutation	UNP Q8WSF8
I	117	TYR	PHE	engineered mutation	UNP Q8WSF8
I	118	LEU	ILE	engineered mutation	UNP Q8WSF8
I	148	SER	VAL	engineered mutation	UNP Q8WSF8
I	186	ARG	GLN	engineered mutation	UNP Q8WSF8
I	187	PHE	HIS	engineered mutation	UNP Q8WSF8
I	189	GLU	SER	engineered mutation	UNP Q8WSF8
I	192	LYS	PRO	engineered mutation	UNP Q8WSF8
I	196	PRO	ILE	engineered mutation	UNP Q8WSF8
I	220	SER	-	expression tag	UNP Q8WSF8
I	221	ARG	-	expression tag	UNP Q8WSF8
J	-8	ASP	-	expression tag	UNP Q8WSF8
J	-7	TYR	-	expression tag	UNP Q8WSF8
J	-6	LYS	-	expression tag	UNP Q8WSF8
J	-5	ASP	-	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
J	55	TRP	TYR	engineered mutation	UNP Q8WSF8
J	106	ASN	ILE	engineered mutation	UNP Q8WSF8
J	108	LEU	VAL	engineered mutation	UNP Q8WSF8

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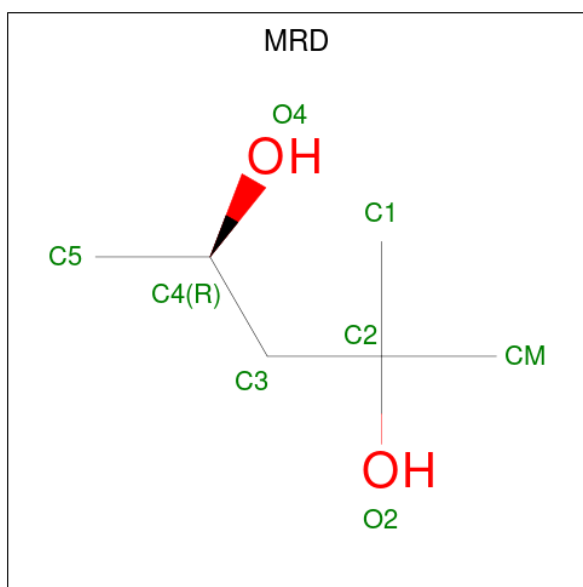
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Chain	Residue	Modelled	Actual	Comment	Reference
J	116	GLN	MET	engineered mutation	UNP Q8WSF8
J	117	TYR	PHE	engineered mutation	UNP Q8WSF8
J	118	LEU	ILE	engineered mutation	UNP Q8WSF8
J	148	SER	VAL	engineered mutation	UNP Q8WSF8
J	186	ARG	GLN	engineered mutation	UNP Q8WSF8
J	187	PHE	HIS	engineered mutation	UNP Q8WSF8
J	189	GLU	SER	engineered mutation	UNP Q8WSF8
J	192	LYS	PRO	engineered mutation	UNP Q8WSF8
J	196	PRO	ILE	engineered mutation	UNP Q8WSF8
J	220	SER	-	expression tag	UNP Q8WSF8
J	221	ARG	-	expression tag	UNP Q8WSF8

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

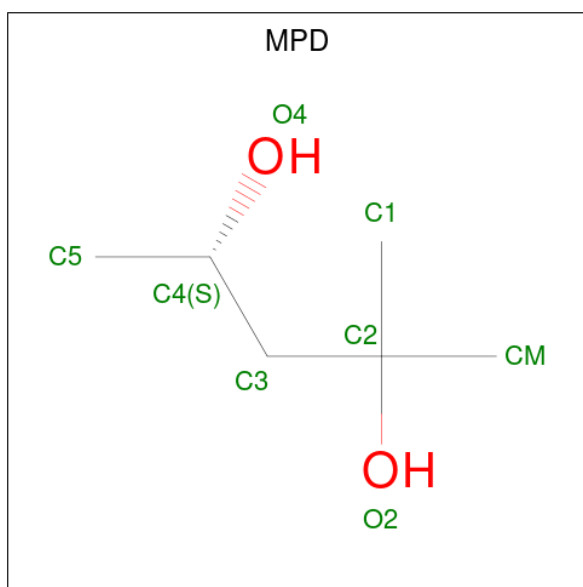
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



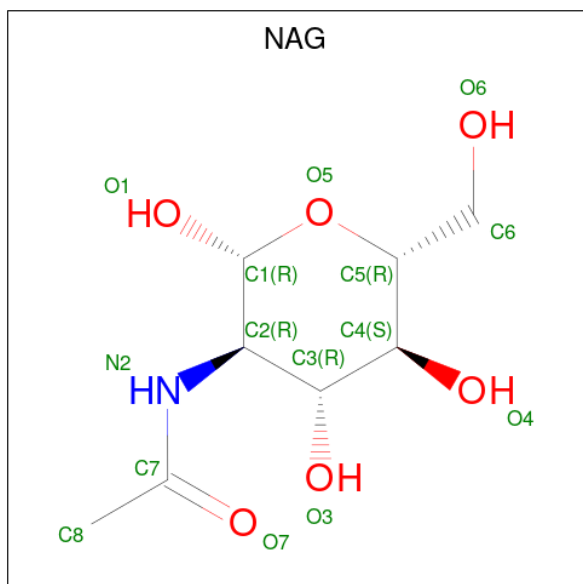
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	I	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	1
			28	16	2	10		

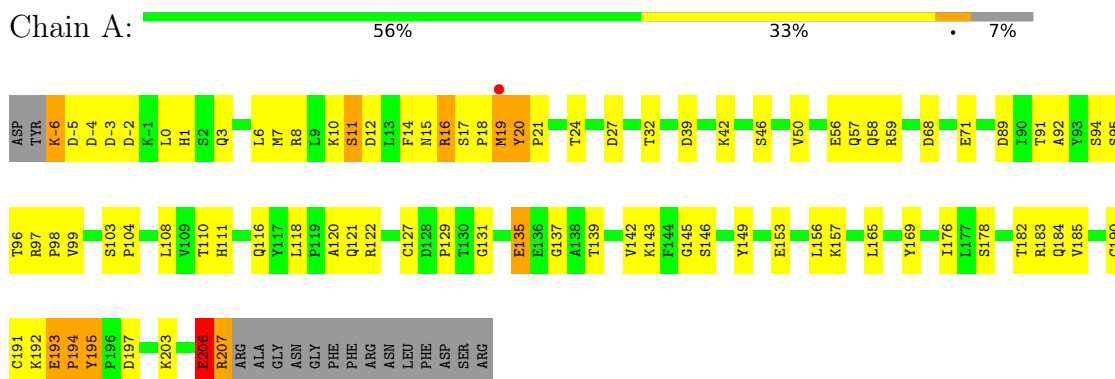
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	B	10	Total O 10 10	0	0
6	C	12	Total O 12 12	0	0
6	D	20	Total O 20 20	0	0
6	E	11	Total O 11 11	0	0
6	F	14	Total O 14 14	0	0
6	G	5	Total O 5 5	0	0
6	H	3	Total O 3 3	0	0
6	I	3	Total O 3 3	0	0
6	J	5	Total O 5 5	0	0

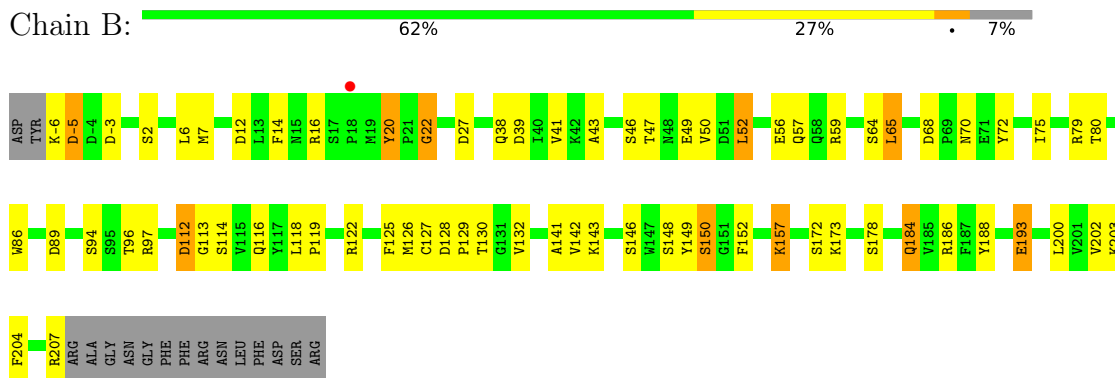
3 Residue-property plots [i](#)

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.

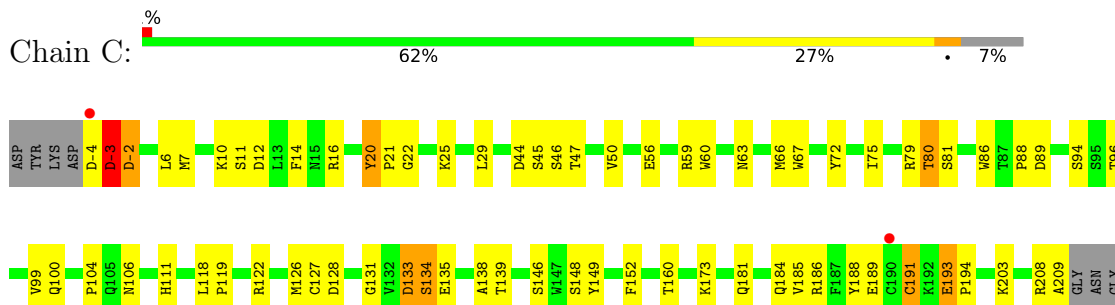
• Molecule 1: Soluble acetylcholine receptor



• Molecule 1: Soluble acetylcholine receptor



• Molecule 1: Soluble acetylcholine receptor



PHE
PHE
ARG
ASN
LEU
PHE
ASP
SER
ARG

• Molecule 1: Soluble acetylcholine receptor

Chain D:  2% 56% 33% 7%

ASP TYR K-6 D-5 D-4 D-3 D-2 K-1 L0 H1 L6 M7 L13 F14 S17 P18 Y20 P21 G22 P23 T24 K25 D26 Q38 D39 T47 R46 E49 V50 D51 L52 E56 Q57 Q58 R59 W60 K61 L62 N63 M65 W67 E71 Y72 G73 N74 I75 T76 D77 F78 R79 T80

S81 T85 A92 Y93 S94 S95 T96 R97 P98 V99 S103 D112 G113 S114 Y115 Q116 Y117 P118 L118 G119 A120 T121 R122 F125 M126 C127 P128 T129 T130 V132 E135 S146 W147 Y148 Y149 I154 D155 L156 D159 Q162 Y163 L165 S166 Y169 S172 K173 Y174

E175 I176 L177 T180 Q181 T182 R183 Q184 C190 C191 K192 E193 D197 R205 E206 R208 ALA G22 ASN GLY PHE PHE ASN LEU PHE ASP ASP ARG

• Molecule 1: Soluble acetylcholine receptor

Chain E:  53% 33% 6% 7%

ASP TYR K-6 N5 L6 M7 R8 L9 S11 L12 L13 F14 N15 R16 P17 S18 M19 Y20 P21 G22 P23 T24 K25 D26 D27 P28 L37 I40 D44 S46 V50 D51 L52 E56 Q57 L62 N63 S64 M66 N70 E71 Y72 G73 R79 T80 W86 T87

P88 D89 T91 S95 T96 R97 P98 Q100 P104 Q105 M106 A107 L108 L118 P119 R122 L123 S124 F125 M126 C127 D128 T129 V130 S131 D132 D133 O134 G140 A141 V142 K143 F144 W147 S148 Y149 I154 Y169 A170 S171 K173 I176 V185 E189 C190

C191 K192 E193 P194 Y195 P196 V201 R205 E206 ARG P104 Q105 M106 A107 L108 L118 P119 R122 L123 S124 F125 M126 C127 D128 T129 V130 S131 D132 D133 O134 G140 A141 V142 K143 F144 W147 S148 Y149 I154 Y169 A170 S171 K173 I176 V185 E189 C190

• Molecule 1: Soluble acetylcholine receptor

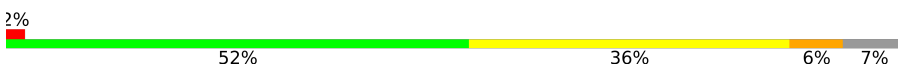
Chain F:  60% 29% 7%

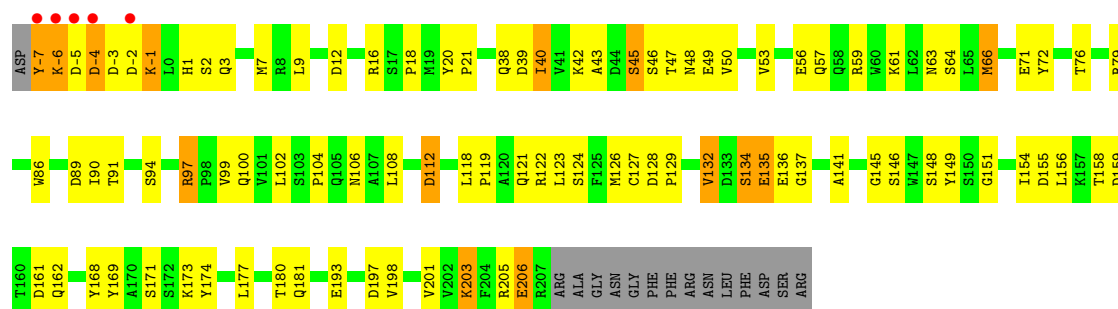
ASP TYR K-6 D-5 Q3 A4 R5 L6 M7 F14 N15 R16 S17 P18 M19 Y20 P21 K25 D26 D27 L33 D44 S45 S46 V50 K61 S64 E71 N74 I90 T91 S94 S95 T96 R97 P98 P104 Q105 N106 T110 H111 D112 Q116 Y117

L123 S124 T125 M126 C127 D128 T129 T130 G131 V132 D133 S134 E135 T139 C140 A141 V142 K143 S148 Y149 S150 G151 F152 E153 T154 D155 L156 Y169 A170 S171 K173 Y174 Q184 V185 R186 E189 E193 P194 Y195 P196 D197 V198 V201 V202 K203 F204 R205 E206 R207 ARG ALA GLY

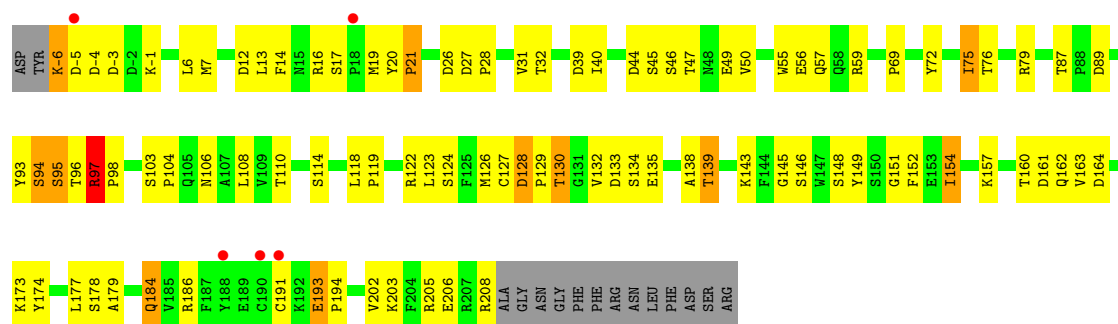
ASN GLY PHE ARG ASN LEU PHE ASP SER ARG

• Molecule 1: Soluble acetylcholine receptor

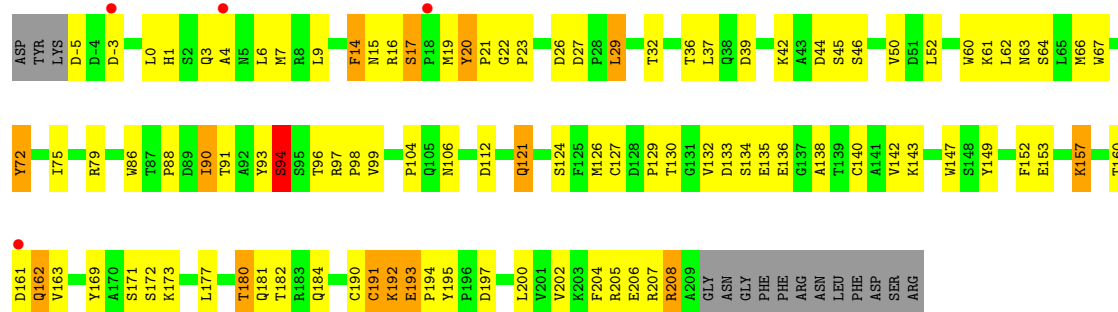
Chain G:  2% 52% 36% 6% 7%



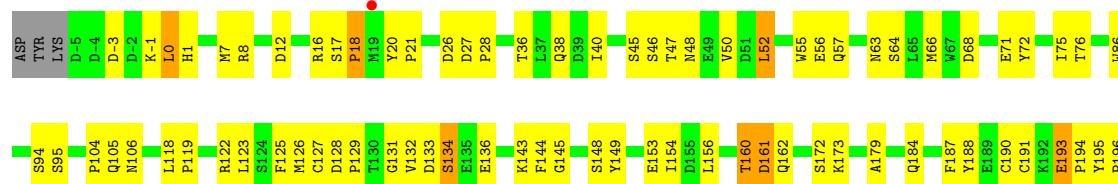
• Molecule 1: Soluble acetylcholine receptor



• Molecule 1: Soluble acetylcholine receptor



• Molecule 1: Soluble acetylcholine receptor



D197		V201		E206	R207	ARG	ALA	GLY	ASN	GLY	PHE	PHE	ARG	ASN	LEU	PHE	ASP	SER	ARG
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.92Å 152.22Å 176.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.20 – 3.00 37.20 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (37.20-3.00) 85.7 (37.20-3.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.189 , 0.240 0.190 , 0.248	Depositor DCC
R_{free} test set	3006 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17570	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.13% 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: MRD, MPD, NAG, CA

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	0.83	4/1781 (0.2%)	1.08	12/2425 (0.5%)
1	B	0.83	3/1767 (0.2%)	1.14	15/2407 (0.6%)
1	C	0.84	2/1769 (0.1%)	1.15	16/2410 (0.7%)
1	D	0.84	4/1787 (0.2%)	1.15	15/2433 (0.6%)
1	E	0.95	5/1779 (0.3%)	1.20	20/2423 (0.8%)
1	F	0.80	1/1789 (0.1%)	1.11	13/2436 (0.5%)
1	G	0.79	3/1783 (0.2%)	1.11	16/2429 (0.7%)
1	H	0.85	4/1795 (0.2%)	1.11	13/2444 (0.5%)
1	I	0.79	3/1807 (0.2%)	1.14	16/2459 (0.7%)
1	J	0.86	2/1787 (0.1%)	1.10	12/2434 (0.5%)
All	All	0.84	31/17844 (0.2%)	1.13	148/24300 (0.6%)

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	92	ALA	C-N	-9.28	1.21	1.33
1	J	195	TYR	C-O	-9.19	1.17	1.25
1	A	92	ALA	C-N	-7.79	1.22	1.33
1	I	90	ILE	CA-CB	-7.46	1.45	1.54
1	A	194	PRO	C-N	-7.46	1.24	1.33

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	16	ARG	N-CA-C	-9.80	100.87	113.12
1	E	195	TYR	CA-C-N	-8.70	111.91	120.52
1	E	195	TYR	C-N-CA	-8.70	111.91	120.52
1	I	17	SER	N-CA-C	8.17	121.45	109.04
1	I	17	SER	CB-CA-C	-8.15	100.55	109.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1733	0	1658	76	0
1	B	1722	0	1636	59	0
1	C	1724	0	1646	62	0
1	D	1739	0	1663	68	0
1	E	1731	0	1655	90	0
1	F	1738	0	1664	74	0
1	G	1737	0	1654	104	0
1	H	1744	0	1669	111	0
1	I	1753	0	1685	96	0
1	J	1733	0	1650	64	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	J	1	0	0	0	0
3	A	8	0	14	1	0
3	B	8	0	14	2	0
3	D	8	0	14	3	0
3	E	8	0	14	1	0
3	F	8	0	14	1	0
3	G	8	0	14	1	0
3	H	16	0	28	6	0
3	I	8	0	14	4	0
4	B	8	0	14	4	0
4	G	8	0	14	4	0
5	F	28	0	26	5	0
6	A	8	0	0	0	0
6	B	10	0	0	0	0
6	C	12	0	0	0	0
6	D	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	11	0	0	3	0
6	F	14	0	0	0	0
6	G	5	0	0	1	0
6	H	3	0	0	0	0
6	I	3	0	0	0	0
6	J	5	0	0	0	0
All	All	17570	0	16760	692	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 20.

The worst 5 of 692 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:I:160:THR:HG22	1:I:162:GLN:H	1.04	1.10
1:D:24:THR:HG22	1:D:26:ASP:H	1.09	1.09
1:J:160:THR:HG22	1:J:162:GLN:H	1.08	1.07
1:F:104:PRO:HD3	1:G:91:THR:HG21	1.36	1.07
1:I:7[A]:MET:HE2	1:J:18:PRO:HB2	1.38	1.05

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	214/230 (93%)	209 (98%)	5 (2%)	0	100	100
1	B	213/230 (93%)	210 (99%)	3 (1%)	0	100	100
1	C	213/230 (93%)	212 (100%)	1 (0%)	0	100	100
1	D	215/230 (94%)	214 (100%)	1 (0%)	0	100	100
1	E	214/230 (93%)	211 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	215/230 (94%)	213 (99%)	2 (1%)	0	100	100
1	G	214/230 (93%)	209 (98%)	5 (2%)	0	100	100
1	H	216/230 (94%)	214 (99%)	2 (1%)	0	100	100
1	I	217/230 (94%)	216 (100%)	1 (0%)	0	100	100
1	J	215/230 (94%)	215 (100%)	0	0	100	100
All	All	2146/2300 (93%)	2123 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	197/208 (95%)	187 (95%)	10 (5%)	21	55
1	B	196/208 (94%)	187 (95%)	9 (5%)	24	58
1	C	195/208 (94%)	186 (95%)	9 (5%)	24	58
1	D	198/208 (95%)	184 (93%)	14 (7%)	13	43
1	E	197/208 (95%)	186 (94%)	11 (6%)	19	52
1	F	198/208 (95%)	189 (96%)	9 (4%)	24	59
1	G	197/208 (95%)	177 (90%)	20 (10%)	7	29
1	H	199/208 (96%)	184 (92%)	15 (8%)	12	41
1	I	199/208 (96%)	185 (93%)	14 (7%)	14	44
1	J	198/208 (95%)	184 (93%)	14 (7%)	13	43
All	All	1974/2080 (95%)	1849 (94%)	125 (6%)	16	48

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	91	THR
1	I	208	ARG

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Mol	Chain	Res	Type
1	G	76	THR
1	I	202	VAL
1	J	105	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	116	GLN
1	J	48	ASN
1	G	38	GLN
1	J	184	GLN
1	I	48	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 9 are monoatomic - leaving 13 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	$\# Z > 2$
4	MPD	B	275	-	7,7,7	0.45	0	9,10,10	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	F	250[B]	-	14,14,15	0.47	0	17,19,21	0.80	0
3	MRD	H	276	-	7,7,7	0.32	0	9,10,10	0.55	0
5	NAG	F	250[A]	-	14,14,15	0.52	0	17,19,21	1.31	2 (11%)
3	MRD	G	222	-	7,7,7	0.29	0	9,10,10	0.45	0
4	MPD	G	275	-	7,7,7	0.40	0	9,10,10	0.75	1 (11%)
3	MRD	D	275	-	7,7,7	0.40	0	9,10,10	0.45	0
3	MRD	H	275	-	7,7,7	0.33	0	9,10,10	0.34	0
3	MRD	E	275	-	7,7,7	0.40	0	9,10,10	0.37	0
3	MRD	B	222	-	7,7,7	0.23	0	9,10,10	0.39	0
3	MRD	F	275	-	7,7,7	0.31	0	9,10,10	0.31	0
3	MRD	A	275	-	7,7,7	0.35	0	9,10,10	0.45	0
3	MRD	I	275	-	7,7,7	0.29	0	9,10,10	0.34	0

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
4	MPD	B	275	-	-	4/5/5/5	-
5	NAG	F	250[B]	-	-	2/6/23/26	0/1/1/1
3	MRD	H	276	-	-	3/5/5/5	-
5	NAG	F	250[A]	-	-	2/6/23/26	0/1/1/1
3	MRD	G	222	-	-	5/5/5/5	-
4	MPD	G	275	-	-	3/5/5/5	-
3	MRD	D	275	-	-	5/5/5/5	-
3	MRD	H	275	-	-	3/5/5/5	-
3	MRD	E	275	-	-	1/5/5/5	-
3	MRD	B	222	-	-	5/5/5/5	-
3	MRD	F	275	-	-	4/5/5/5	-
3	MRD	A	275	-	-	3/5/5/5	-
3	MRD	I	275	-	-	4/5/5/5	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	250[A]	NAG	O5-C1-C2	-3.55	105.80	111.29
5	F	250[A]	NAG	C3-C4-C5	2.55	114.86	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	G	275	MPD	CM-C2-C1	2.04	115.20	110.63

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	275	MRD	C2-C3-C4-O4
3	D	275	MRD	C2-C3-C4-C5
3	F	275	MRD	C1-C2-C3-C4
3	F	275	MRD	O2-C2-C3-C4
3	G	222	MRD	C1-C2-C3-C4

There are no ring outliers.

13 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	275	MPD	4	0
5	F	250[B]	NAG	1	0
3	H	276	MRD	3	0
5	F	250[A]	NAG	4	0
3	G	222	MRD	1	0
4	G	275	MPD	4	0
3	D	275	MRD	3	0
3	H	275	MRD	3	0
3	E	275	MRD	1	0
3	B	222	MRD	2	0
3	F	275	MRD	1	0
3	A	275	MRD	1	0
3	I	275	MRD	4	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 ⓘ

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	214/230 (93%)	-0.27	1 (0%)	87 72	12, 31, 74, 92	2 (0%)
1	B	214/230 (93%)	-0.34	1 (0%)	87 72	13, 28, 60, 86	1 (0%)
1	C	214/230 (93%)	-0.37	2 (0%)	81 61	11, 27, 72, 89	1 (0%)
1	D	215/230 (93%)	-0.38	4 (1%)	66 43	11, 26, 66, 88	2 (0%)
1	E	214/230 (93%)	-0.34	1 (0%)	87 72	14, 28, 67, 91	2 (0%)
1	F	214/230 (93%)	-0.31	2 (0%)	81 61	13, 30, 67, 88	3 (1%)
1	G	215/230 (93%)	-0.17	5 (2%)	61 38	14, 34, 74, 107	1 (0%)
1	H	215/230 (93%)	0.03	5 (2%)	61 38	16, 41, 79, 103	3 (1%)
1	I	215/230 (93%)	0.03	4 (1%)	66 43	15, 39, 85, 105	4 (1%)
1	J	213/230 (92%)	-0.28	1 (0%)	87 72	19, 31, 76, 95	4 (1%)
All	All	2143/2300 (93%)	-0.24	26 (1%)	76 55	11, 32, 72, 107	23 (1%)

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	-4	ASP	6.2
1	I	18	PRO	3.4
1	H	18	PRO	3.0
1	B	18	PRO	2.8
1	H	188	TYR	2.8

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 [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	MRD	H	276	8/8	0.74	0.23	56,66,75,76	0
5	NAG	F	250[A]	14/15	0.77	0.16	38,52,58,60	14
5	NAG	F	250[B]	14/15	0.77	0.16	48,54,59,59	14
2	CA	D	225	1/1	0.81	0.18	98,98,98,98	0
3	MRD	H	275	8/8	0.82	0.16	47,59,68,68	0
3	MRD	B	222	8/8	0.86	0.21	38,44,61,64	0
2	CA	B	225	1/1	0.87	0.12	80,80,80,80	0
4	MPD	G	275	8/8	0.88	0.15	32,45,54,64	0
3	MRD	A	275	8/8	0.88	0.12	41,43,67,70	0
2	CA	E	225	1/1	0.88	0.12	81,81,81,81	0
3	MRD	E	275	8/8	0.89	0.12	28,45,53,54	0
3	MRD	F	275	8/8	0.89	0.15	39,43,60,61	0
3	MRD	I	275	8/8	0.89	0.13	32,44,54,62	0
2	CA	J	225	1/1	0.90	0.12	72,72,72,72	0
2	CA	H	225	1/1	0.92	0.13	76,76,76,76	0
3	MRD	G	222	8/8	0.93	0.11	46,54,60,62	0
4	MPD	B	275	8/8	0.94	0.10	30,41,50,53	0
2	CA	A	225	1/1	0.95	0.13	77,77,77,77	0
3	MRD	D	275	8/8	0.95	0.11	28,35,47,66	0
2	CA	G	225	1/1	0.96	0.19	77,77,77,77	0
2	CA	C	225	1/1	0.98	0.09	65,65,65,65	0
2	CA	F	225	1/1	0.98	0.07	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.