wwPDB X-ray Structure Validation Summary Report (i)

Mar 23, 2024 – 02:15 PM EDT

PDB ID	:	3T4M
Title	:	Ac-AChBP ligand binding domain mutated to human alpha-7 nAChR (intermediate)
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 (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:

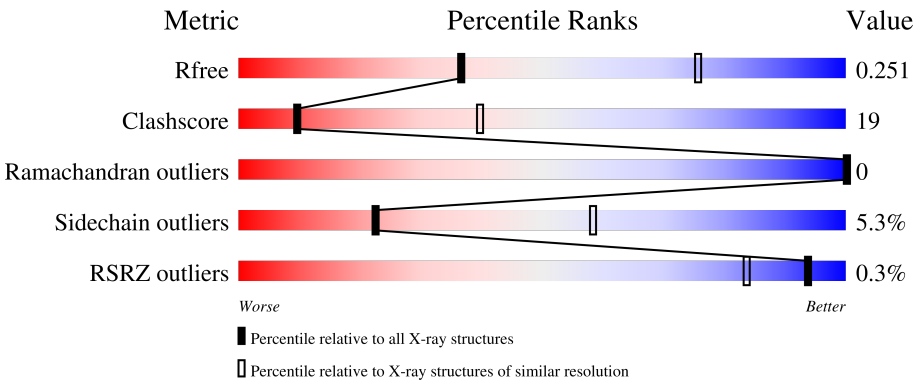
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	58% 32% • 7%
1	B	230	65% 27% • 7%
1	C	230	67% 24% • 7%
1	D	230	58% 33% • 7%
1	E	230	56% 33% • 7%

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Mol	Chain	Length	Quality of chain
1	F	230	65% 25% • 7%
1	G	230	2% 57% 34% • 7%
1	H	230	58% 32% • 7%
1	I	230	53% 36% • 7%
1	J	230	60% 33% 7%

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
5	NAG	F	250[A]	-	-	-	X
5	NAG	F	250[B]	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	214	1733	1090	289	346	8	0	2	0
1	B	214	1722	1083	283	348	8	0	1	0
1	C	214	1724	1084	288	344	8	0	1	0
1	D	215	1739	1093	290	348	8	0	2	0
1	E	214	1731	1089	287	347	8	0	2	0
1	F	214	1738	1093	290	347	8	0	3	0
1	G	215	1737	1094	287	348	8	0	1	0
1	H	215	1744	1096	291	349	8	0	3	0
1	I	215	1753	1102	295	347	9	0	4	0
1	J	213	1733	1090	285	350	8	0	4	0

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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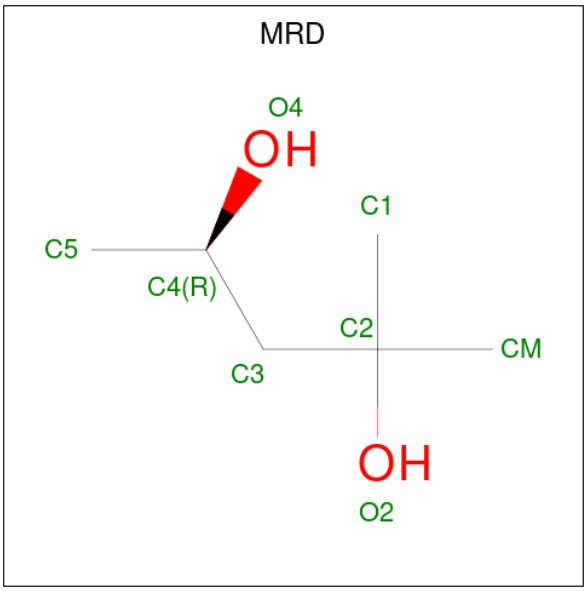
Chain	Residue	Modelled	Actual	Comment	Reference
J	116	GLN	MET	engineered mutation	UNP Q8WSF8
J	117	TYR	PHE	engineered mutation	UNP Q8WSF8
J	118	LEU	ILE	engineered mutation	UNP Q8WSF8
J	148	SER	VAL	engineered mutation	UNP Q8WSF8
J	186	ARG	GLN	engineered mutation	UNP Q8WSF8
J	187	PHE	HIS	engineered mutation	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 (three-letter code: CA) (formula: Ca).

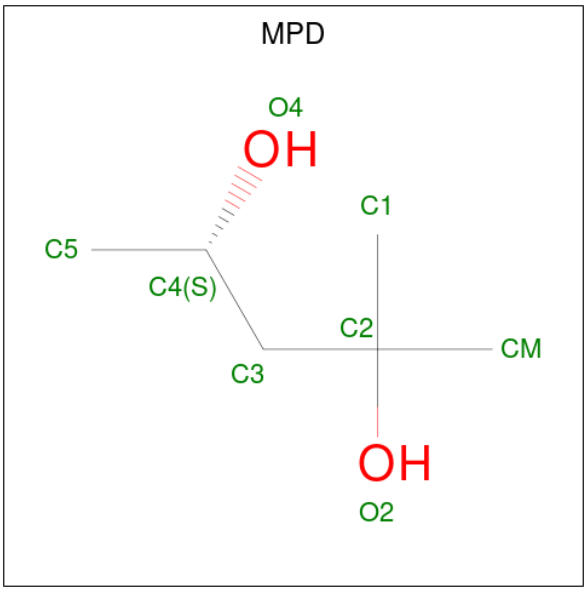
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0
2	G	1	1	1	0	0
2	H	1	1	1	0	0
2	J	1	1	1	0	0

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



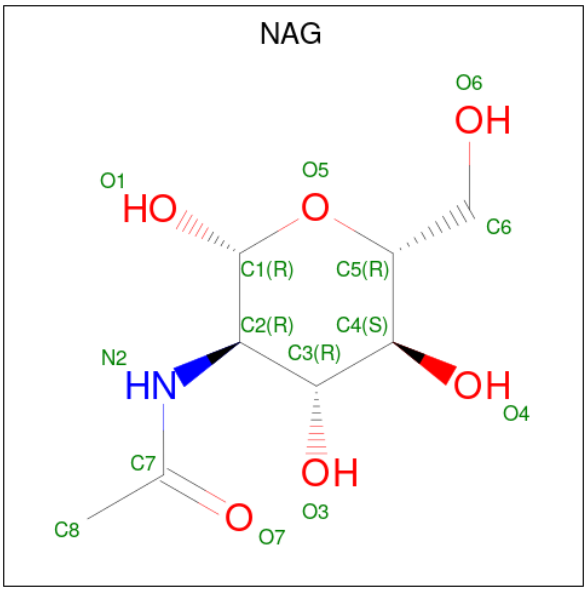
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	8	6	2	0	0
3	B	1	8	6	2	0	0
3	D	1	8	6	2	0	0
3	E	1	8	6	2	0	0
3	F	1	8	6	2	0	0
3	G	1	8	6	2	0	0
3	H	1	8	6	2	0	0
3	H	1	8	6	2	0	0
3	I	1	8	6	2	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

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



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

- Molecule 6 is water.

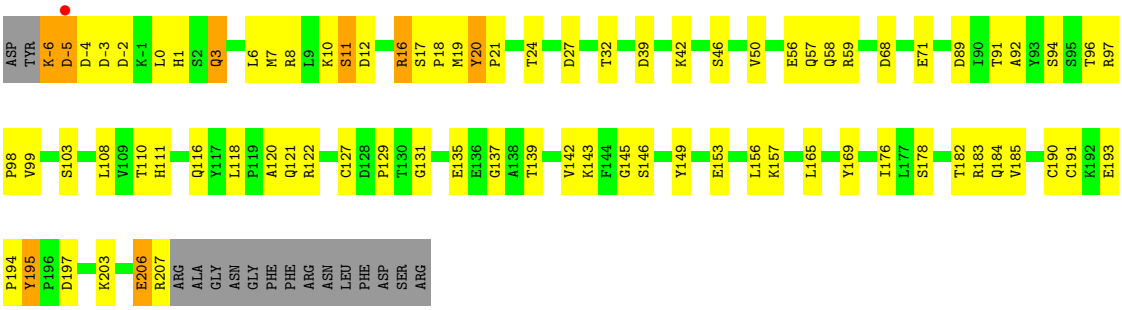
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	B	10	Total O 10 10	0	0
6	C	12	Total O 12 12	0	0
6	D	20	Total O 20 20	0	0
6	E	11	Total O 11 11	0	0
6	F	14	Total O 14 14	0	0
6	G	5	Total O 5 5	0	0
6	H	3	Total O 3 3	0	0
6	I	3	Total O 3 3	0	0
6	J	5	Total O 5 5	0	0

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.

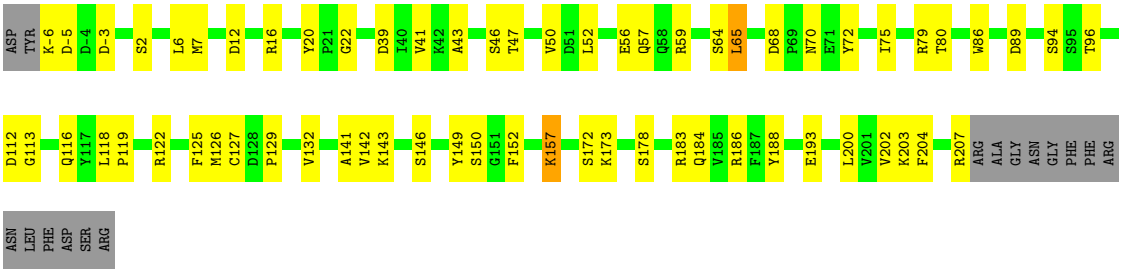
• Molecule 1: Soluble acetylcholine receptor

Chain A: 58% 32% • 7%



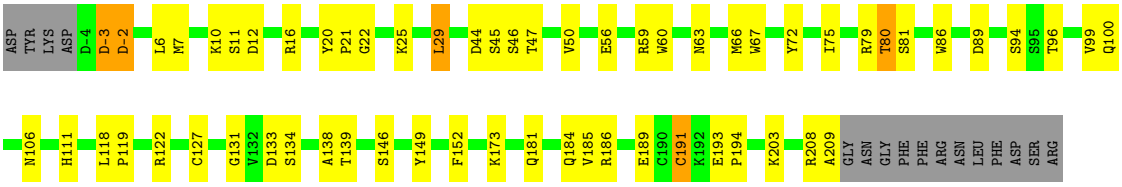
• Molecule 1: Soluble acetylcholine receptor

Chain B: 65% 27% • 7%



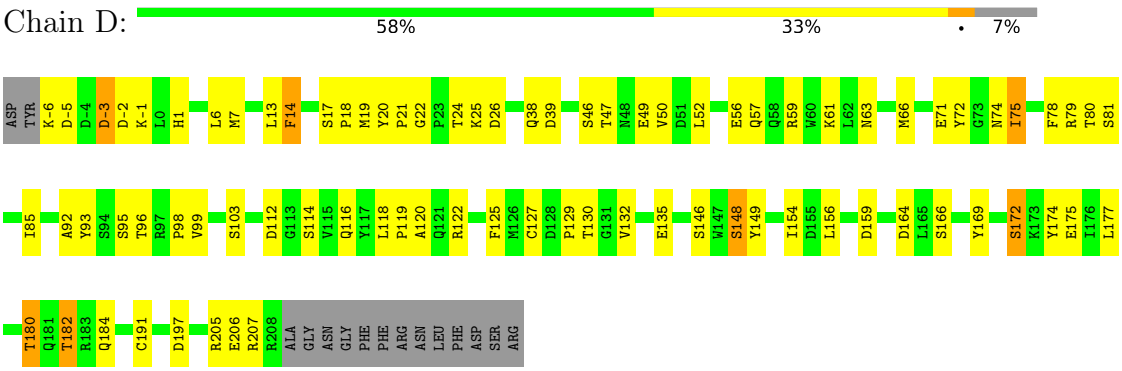
• Molecule 1: Soluble acetylcholine receptor

Chain C: 67% 24% • 7%



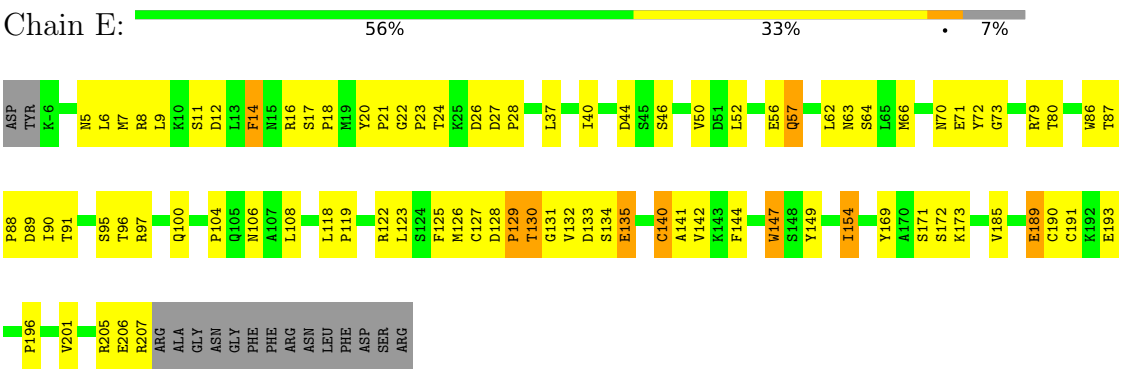
• Molecule 1: Soluble acetylcholine receptor

Chain D:



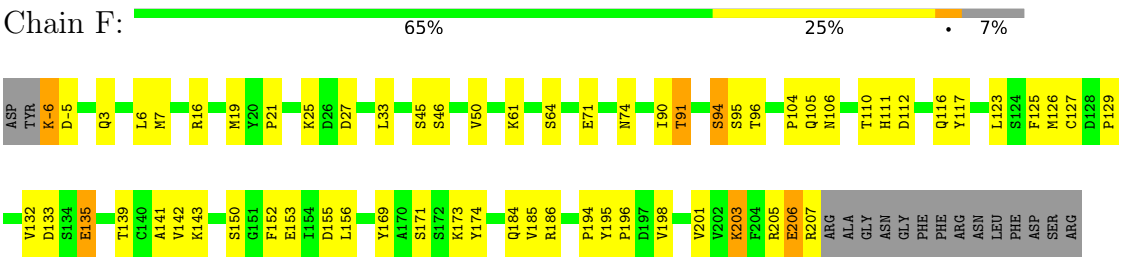
• Molecule 1: Soluble acetylcholine receptor

Chain E:



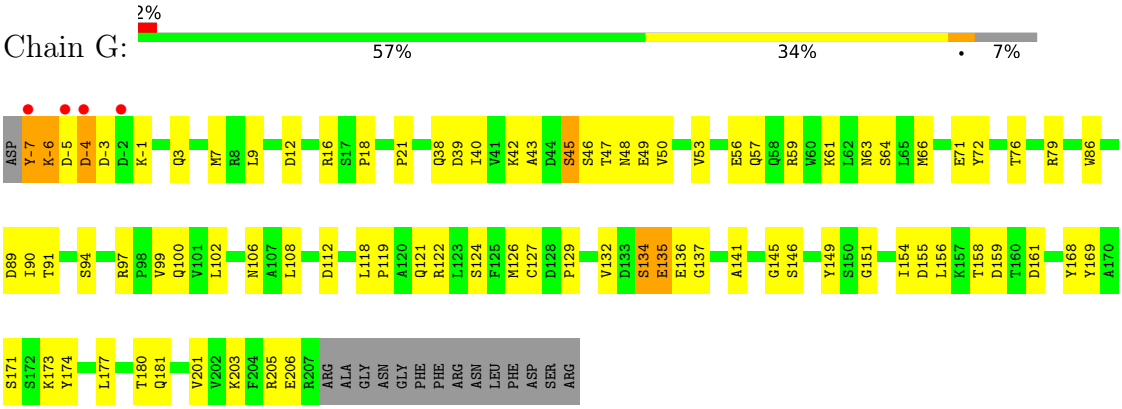
• Molecule 1: Soluble acetylcholine receptor

Chain F:



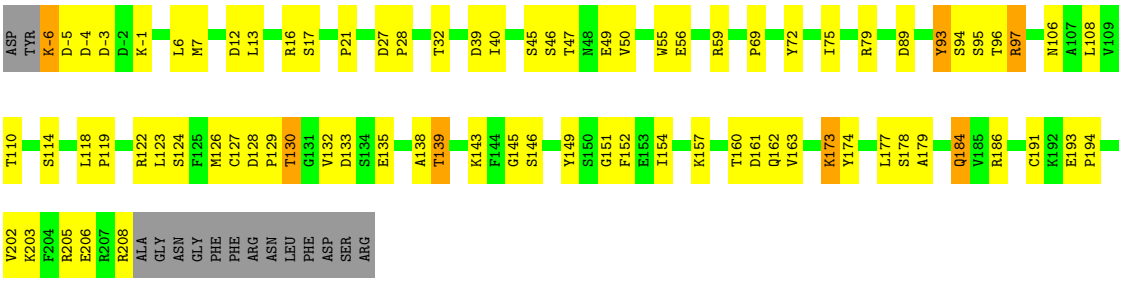
• Molecule 1: Soluble acetylcholine receptor

Chain G:



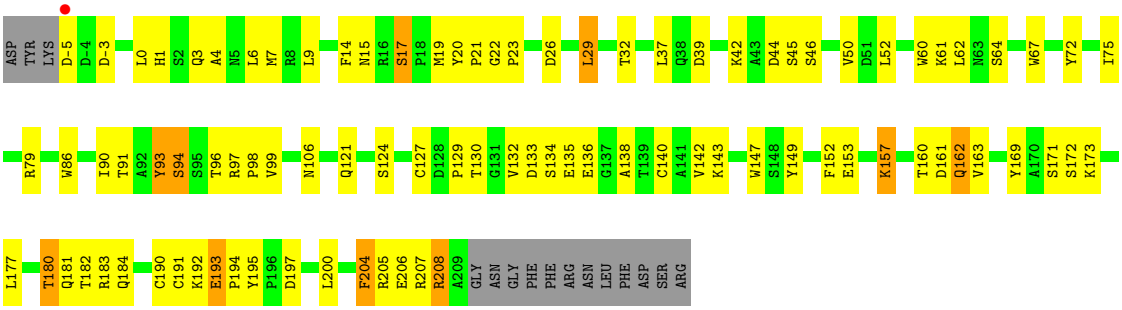
• Molecule 1: Soluble acetylcholine receptor

Chain H:



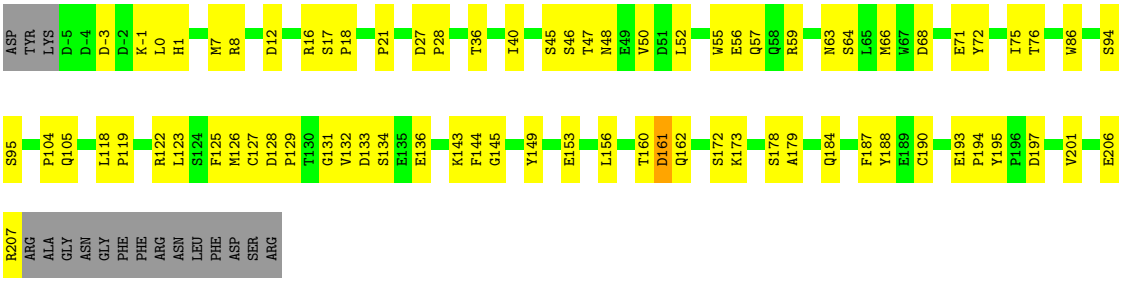
- Molecule 1: Soluble acetylcholine receptor

Chain I:



- Molecule 1: Soluble acetylcholine receptor

Chain J:



4 Data and refinement statistics (i)

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 45.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (37.20-3.00) 94.3 (45.99-3.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.22	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.189 , 0.240 0.192 , 0.251	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 , 35.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MPD, CA, MRD

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	0.66	1/1781 (0.1%)	0.78	3/2425 (0.1%)
1	B	0.68	0/1767	0.77	0/2407
1	C	0.69	0/1769	0.80	1/2410 (0.0%)
1	D	0.66	1/1787 (0.1%)	0.76	2/2433 (0.1%)
1	E	0.78	3/1779 (0.2%)	0.79	1/2423 (0.0%)
1	F	0.63	0/1789	0.75	1/2436 (0.0%)
1	G	0.65	0/1783	0.77	0/2429
1	H	0.71	1/1795 (0.1%)	0.75	0/2444
1	I	0.65	1/1807 (0.1%)	0.74	1/2459 (0.0%)
1	J	0.71	1/1787 (0.1%)	0.77	0/2434
All	All	0.68	8/17844 (0.0%)	0.77	9/24300 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	140	CYS	CB-SG	-5.83	1.72	1.81
1	J	195	TYR	CE2-CZ	-5.75	1.31	1.38
1	H	93	TYR	CE2-CZ	-5.63	1.31	1.38
1	D	92	ALA	C-N	-5.62	1.21	1.34
1	I	93	TYR	CE2-CZ	-5.34	1.31	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	206	GLU	CB-CA-C	-5.86	98.69	110.40
1	E	14	PHE	CB-CA-C	-5.84	98.72	110.40
1	F	206	GLU	CB-CA-C	-5.81	98.78	110.40
1	C	29	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	195	TYR	CB-CG-CD1	-5.42	117.75	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1733	0	1658	73	0
1	B	1722	0	1636	54	0
1	C	1724	0	1646	59	0
1	D	1739	0	1662	62	0
1	E	1731	0	1655	83	0
1	F	1738	0	1664	74	0
1	G	1737	0	1654	100	0
1	H	1744	0	1669	103	0
1	I	1753	0	1685	91	0
1	J	1733	0	1650	67	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	3	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	16759	663	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 19.

The worst 5 of 663 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:143:LYS:HE2	1:I:184:GLN:HE22	1.23	1.02

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 (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	197/208 (95%)	186 (94%)	11 (6%)	21	56
1	B	196/208 (94%)	189 (96%)	7 (4%)	35	70
1	C	195/208 (94%)	187 (96%)	8 (4%)	30	67
1	D	198/208 (95%)	184 (93%)	14 (7%)	14	46
1	E	197/208 (95%)	187 (95%)	10 (5%)	24	60
1	F	198/208 (95%)	191 (96%)	7 (4%)	36	71
1	G	197/208 (95%)	184 (93%)	13 (7%)	16	49
1	H	199/208 (96%)	188 (94%)	11 (6%)	21	57
1	I	199/208 (96%)	186 (94%)	13 (6%)	17	50
1	J	198/208 (95%)	184 (93%)	14 (7%)	14	46
All	All	1974/2080 (95%)	1866 (94%)	108 (6%)	22	57

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	-7	TYR
1	H	-5	ASP

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Mol	Chain	Res	Type
1	J	76	THR
1	G	-4	ASP
1	G	94	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	57	GLN
1	G	105	GLN
1	J	184	GLN
1	G	100	GLN
1	G	184	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)

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	0.42	0	9,10,10	0.56	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	0.49	0	17,19,21	0.84	0
3	MRD	H	276	-	7,7,7	0.33	0	9,10,10	0.56	0
3	MRD	F	275	-	7,7,7	0.29	0	9,10,10	0.28	0
5	NAG	F	250[A]	-	14,14,15	0.54	0	17,19,21	1.33	2 (11%)
3	MRD	E	275	-	7,7,7	0.39	0	9,10,10	0.39	0
3	MRD	B	222	-	7,7,7	0.20	0	9,10,10	0.35	0
3	MRD	A	275	-	7,7,7	0.32	0	9,10,10	0.44	0
3	MRD	I	275	-	7,7,7	0.27	0	9,10,10	0.32	0
3	MRD	H	275	-	7,7,7	0.31	0	9,10,10	0.36	0
4	MPD	G	275	-	7,7,7	0.35	0	9,10,10	0.81	1 (11%)
3	MRD	G	222	-	7,7,7	0.28	0	9,10,10	0.42	0
3	MRD	D	275	-	7,7,7	0.36	0	9,10,10	0.43	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	-	-	2/5/5/5	-
3	MRD	F	275	-	-	4/5/5/5	-
5	NAG	F	250[A]	-	-	2/6/23/26	0/1/1/1
3	MRD	E	275	-	-	0/5/5/5	-
3	MRD	B	222	-	-	4/5/5/5	-
3	MRD	A	275	-	-	3/5/5/5	-
3	MRD	I	275	-	-	5/5/5/5	-
3	MRD	H	275	-	-	1/5/5/5	-
4	MPD	G	275	-	-	1/5/5/5	-
3	MRD	G	222	-	-	3/5/5/5	-
3	MRD	D	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(^{o})	Ideal(^{o})
5	F	250[A]	NAG	O5-C1-C2	-3.47	105.80	111.29
5	F	250[A]	NAG	C3-C4-C5	2.59	114.86	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	275	MPD	CM-C2-C1	2.22	115.20	110.57

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

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

There are no ring outliers.

13 monomers are involved in 31 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
3	F	275	MRD	1	0
5	F	250[A]	NAG	4	0
3	E	275	MRD	1	0
3	B	222	MRD	2	0
3	A	275	MRD	1	0
3	I	275	MRD	3	0
3	H	275	MRD	3	0
4	G	275	MPD	4	0
3	G	222	MRD	1	0
3	D	275	MRD	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.58	1 (0%) 91 75	18, 31, 74, 92	0
1	B	214/230 (93%)	-0.66	0 100 100	13, 28, 60, 86	0
1	C	214/230 (93%)	-0.67	0 100 100	15, 27, 72, 89	0
1	D	215/230 (93%)	-0.66	0 100 100	14, 26, 66, 88	0
1	E	214/230 (93%)	-0.67	0 100 100	18, 28, 67, 91	0
1	F	214/230 (93%)	-0.61	0 100 100	19, 30, 67, 88	0
1	G	215/230 (93%)	-0.60	4 (1%) 66 37	20, 34, 74, 107	0
1	H	215/230 (93%)	-0.48	0 100 100	26, 41, 79, 103	0
1	I	215/230 (93%)	-0.38	1 (0%) 91 75	23, 40, 85, 105	0
1	J	213/230 (92%)	-0.57	0 100 100	19, 31, 76, 95	0
All	All	2143/2300 (93%)	-0.59	6 (0%) 94 84	13, 32, 72, 107	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	-4	ASP	3.1
1	A	-5	ASP	2.7
1	I	-5	ASP	2.6
1	G	-7	TYR	2.3
1	G	-5	ASP	2.2

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
5	NAG	F	250[A]	14/15	0.65	0.40	38,52,58,60	14
5	NAG	F	250[B]	14/15	0.65	0.40	48,54,59,59	14
3	MRD	H	276	8/8	0.72	0.25	56,66,75,76	0
3	MRD	E	275	8/8	0.86	0.29	28,45,53,54	0
3	MRD	A	275	8/8	0.87	0.28	41,43,67,70	0
2	CA	G	225	1/1	0.88	0.30	77,77,77,77	0
3	MRD	B	222	8/8	0.88	0.37	38,44,61,64	0
2	CA	D	225	1/1	0.89	0.12	98,98,98,98	0
2	CA	A	225	1/1	0.90	0.14	77,77,77,77	0
3	MRD	H	275	8/8	0.90	0.26	47,59,68,68	0
2	CA	E	225	1/1	0.91	0.22	81,81,81,81	0
3	MRD	F	275	8/8	0.91	0.27	39,43,60,61	0
2	CA	B	225	1/1	0.91	0.22	80,80,80,80	0
3	MRD	I	275	8/8	0.92	0.31	32,44,54,62	0
4	MPD	G	275	8/8	0.92	0.36	32,45,54,64	0
2	CA	H	225	1/1	0.94	0.13	76,76,76,76	0
3	MRD	G	222	8/8	0.94	0.39	46,54,60,62	0
3	MRD	D	275	8/8	0.95	0.26	28,35,47,66	0
2	CA	J	225	1/1	0.95	0.30	72,72,72,72	0
4	MPD	B	275	8/8	0.96	0.31	30,41,50,53	0
2	CA	F	225	1/1	0.96	0.18	62,62,62,62	0
2	CA	C	225	1/1	0.97	0.16	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.