



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:35 AM UTC

PDB ID : 1UV6 / pdb_00001uv6
Title : X-ray structure of acetylcholine binding protein (AChBP) in complex with carbamylcholine
Authors : Celie, P.H.N.; Van Rossum-fikkert, S.E.; Van Dijk, W.J.; Brejc, K.; Smit, A.B.; Sixma, T.K.
Deposited on : 2004-01-15
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

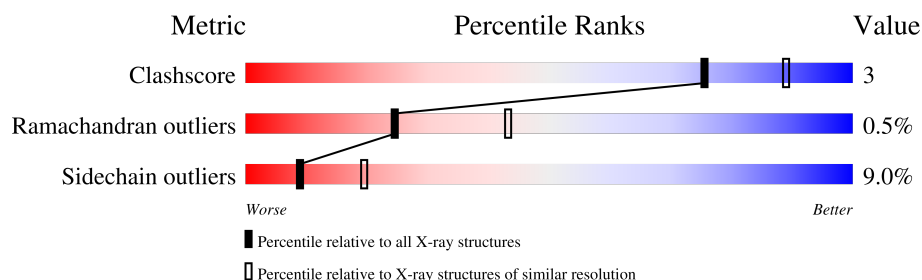
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	210	85% 12% ..
1	B	210	85% 10% ..
1	C	210	85% 11% ..
1	D	210	82% 15% ..
1	E	210	84% 12% ..
1	F	210	80% 14% ..
1	G	210	86% 11% ..
1	H	210	84% 11% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	210	 81%14% ..
1	J	210	 82%14% ..

2 Entry composition

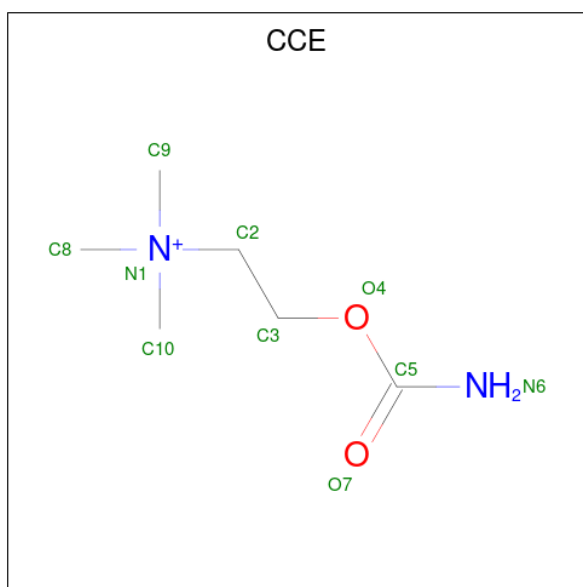
There are 3 unique types of molecules in this entry. The entry contains 16488 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	B	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	C	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	D	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	E	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	F	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	G	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	H	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	I	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			
1	J	205	Total	C	N	O	S	0	0	0
			1636	1023	280	328	5			

- Molecule 2 is 2-[(AMINOCARBONYL)OXY]-N,N,N-TRIMETHYLETHANAMINIUM (CCD ID: CCE) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			10	6	2	2		
2	D	1	Total	C	N	O	0	0
			10	6	2	2		
2	J	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	10	Total	O	0	0
			10	10		
3	C	12	Total	O	0	0
			12	12		
3	D	11	Total	O	0	0
			11	11		
3	E	7	Total	O	0	0
			7	7		
3	F	8	Total	O	0	0
			8	8		
3	G	11	Total	O	0	0
			11	11		
3	H	8	Total	O	0	0
			8	8		
3	I	10	Total	O	0	0
			10	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	8	Total	O	0	0
			8	8		

3 Residue-property plots

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.

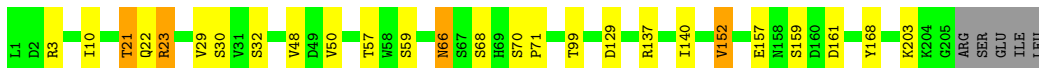
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain A: 



• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain B: 



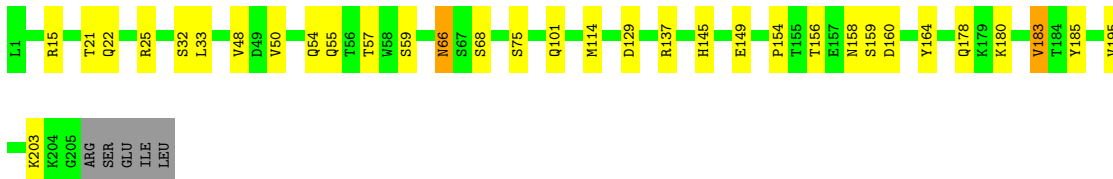
• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain C: 



• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

Chain D: 

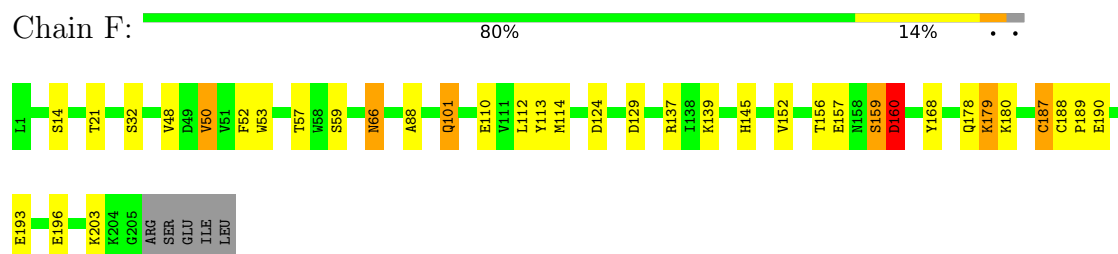


• Molecule 1: ACETYLCHOLINE-BINDING PROTEIN

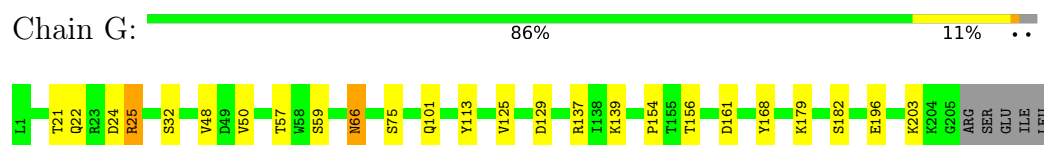
Chain E: 



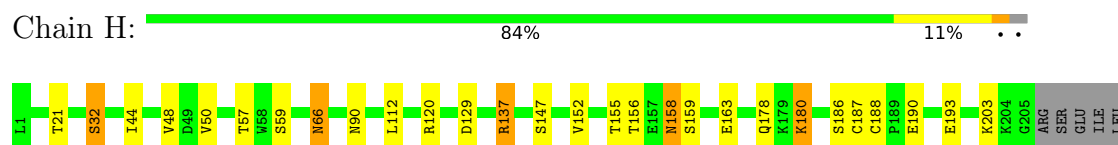
● Molecule 1: ACETYLCHOLINE-BINDING PROTEIN



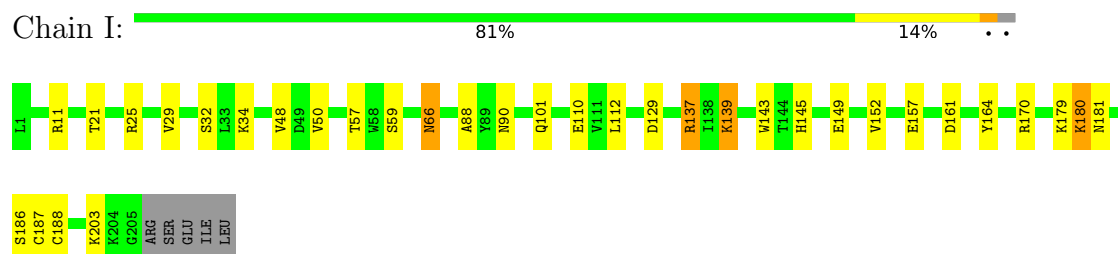
● Molecule 1: ACETYLCHOLINE-BINDING PROTEIN



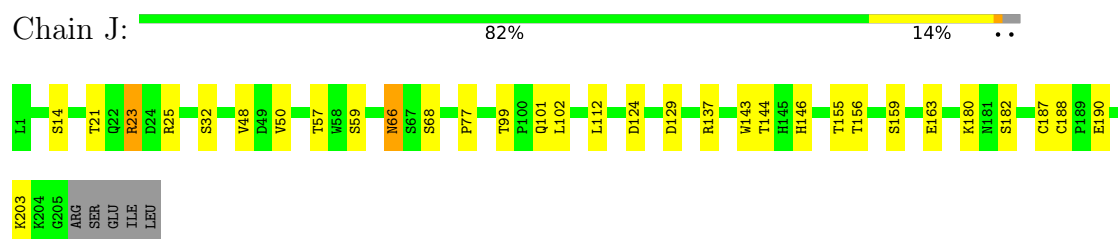
● Molecule 1: ACETYLCHOLINE-BINDING PROTEIN



● Molecule 1: ACETYLCHOLINE-BINDING PROTEIN



● Molecule 1: ACETYLCHOLINE-BINDING PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.90 Å 140.90 Å 240.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.50	Depositor
% Data completeness (in resolution range)	96.3 (12.00-2.50)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.227 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16488	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: CCE

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	0.99	0/1672	0.97	0/2282
1	B	0.93	2/1672 (0.1%)	0.93	0/2282
1	C	0.91	0/1672	0.92	0/2282
1	D	0.93	0/1672	0.97	1/2282 (0.0%)
1	E	0.92	0/1672	0.95	0/2282
1	F	0.93	0/1672	0.93	0/2282
1	G	0.93	0/1672	0.93	0/2282
1	H	0.96	0/1672	0.97	0/2282
1	I	0.93	0/1672	0.92	0/2282
1	J	0.91	0/1672	0.94	0/2282
All	All	0.93	2/16720 (0.0%)	0.94	1/22820 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	ILE	C-O	-5.07	1.18	1.24
1	B	10	ILE	C-O	-5.00	1.18	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	183	VAL	N-CA-C	5.50	115.81	108.11

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	187	CYS	Peptide

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	1636	0	1581	12	0
1	B	1636	0	1581	7	0
1	C	1636	0	1581	9	0
1	D	1636	0	1581	11	0
1	E	1636	0	1581	12	0
1	F	1636	0	1581	20	0
1	G	1636	0	1581	7	0
1	H	1636	0	1581	8	0
1	I	1636	0	1581	13	0
1	J	1636	0	1581	13	0
2	C	10	0	15	0	0
2	D	10	0	15	0	0
2	J	10	0	15	3	0
3	A	13	0	0	1	0
3	B	10	0	0	1	0
3	C	12	0	0	1	0
3	D	11	0	0	0	0
3	E	7	0	0	1	0
3	F	8	0	0	2	0
3	G	11	0	0	0	0
3	H	8	0	0	1	0
3	I	10	0	0	1	0
3	J	8	0	0	1	0
All	All	16488	0	15855	98	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 3.

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:LYS:NZ	1:F:196:GLU:OE1	1.89	1.05
1:C:145:HIS:HE1	1:D:75:SER:HB2	1.52	0.75
1:A:145:HIS:HD2	1:A:149:GLU:OE1	1.71	0.73
1:I:11:ARG:HD3	3:I:2001:HOH:O	1.93	0.67
1:E:155:THR:HG22	1:E:156:THR:HG22	1.75	0.66
1:F:53:TRP:CE3	1:F:114:MET:HE3	2.31	0.65
1:H:120:ARG:NH2	3:H:2006:HOH:O	2.33	0.62
1:A:75:SER:HB2	1:E:145:HIS:HE1	1.65	0.61
1:F:179:LYS:CE	1:F:196:GLU:OE1	2.49	0.60
1:G:101:GLN:NE2	1:G:113:TYR:OH	2.35	0.59
3:A:2004:HOH:O	1:E:15:ARG:HD2	2.02	0.58
1:I:145:HIS:HD2	1:I:149:GLU:OE1	1.86	0.58
1:A:66:ASN:ND2	1:A:68:SER:OG	2.38	0.57
1:C:187:CYS:HB3	3:C:2009:HOH:O	2.04	0.56
1:H:147:SER:HB2	1:H:193:GLU:OE2	2.06	0.55
1:D:145:HIS:HD2	1:D:149:GLU:OE1	1.88	0.55
1:D:55:GLN:HA	1:D:114:MET:HG3	1.88	0.55
1:I:186:SER:OG	1:J:163:GLU:OE1	2.25	0.55
1:A:75:SER:CB	1:E:145:HIS:HE1	2.20	0.55
1:J:77:PRO:HA	1:J:102:LEU:HD23	1.89	0.55
1:F:101:GLN:NE2	1:F:113:TYR:OH	2.41	0.54
1:D:154:PRO:HB3	1:D:195:VAL:HG22	1.90	0.54
1:C:145:HIS:HE1	1:D:75:SER:CB	2.19	0.53
1:C:22:GLN:O	1:C:23:ARG:C	2.52	0.52
1:G:22:GLN:O	1:G:25:ARG:HB2	2.10	0.51
1:J:146:HIS:ND1	1:J:190:GLU:HG3	2.26	0.51
1:E:66:ASN:C	1:E:66:ASN:HD22	2.19	0.50
1:F:168:TYR:CE1	1:J:124:ASP:HB2	2.45	0.50
1:C:77:PRO:HA	1:C:102:LEU:HD23	1.93	0.50
1:H:66:ASN:C	1:H:66:ASN:HD22	2.19	0.50
1:A:187:CYS:SG	1:A:188:CYS:N	2.84	0.49
1:A:75:SER:OG	1:E:145:HIS:CE1	2.66	0.49
1:I:66:ASN:C	1:I:66:ASN:HD22	2.20	0.49
1:I:34:LYS:HD2	1:I:164:TYR:CE2	2.49	0.48
1:E:29:VAL:O	1:E:152:VAL:HA	2.13	0.48
1:F:152:VAL:O	1:F:180:LYS:NZ	2.37	0.48
1:D:156:THR:OG1	1:D:178:GLN:HG3	2.13	0.48
1:F:159:SER:O	1:F:160:ASP:C	2.56	0.48
1:A:152:VAL:HG21	1:A:194:ASP:HA	1.96	0.47
1:J:66:ASN:HD22	1:J:66:ASN:C	2.22	0.47
1:F:66:ASN:HD22	1:F:66:ASN:C	2.22	0.47
1:E:187:CYS:SG	1:E:188:CYS:N	2.88	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:88:ALA:HA	1:I:139:LYS:O	2.15	0.46
1:F:157:GLU:CD	1:F:178:GLN:HG3	2.41	0.46
3:F:2008:HOH:O	1:J:187:CYS:HB3	2.14	0.46
1:F:157:GLU:OE2	1:F:178:GLN:HG3	2.14	0.46
1:E:152:VAL:O	1:E:180:LYS:HD3	2.15	0.46
1:G:66:ASN:C	1:G:66:ASN:HD22	2.24	0.46
1:B:66:ASN:HD22	1:B:66:ASN:C	2.24	0.45
1:J:14:SER:HB3	3:J:2002:HOH:O	2.16	0.44
1:F:187:CYS:SG	1:F:188:CYS:N	2.90	0.44
1:F:145:HIS:CE1	1:G:75:SER:HB2	2.52	0.44
1:I:180:LYS:HD3	1:I:181:ASN:N	2.32	0.44
1:F:188:CYS:O	1:F:190:GLU:N	2.51	0.44
1:H:152:VAL:O	1:H:180:LYS:HE3	2.18	0.44
1:A:146:HIS:CE1	1:A:148:ARG:HB2	2.52	0.44
1:E:11:ARG:HD3	3:E:2001:HOH:O	2.17	0.44
1:F:179:LYS:HE2	1:F:196:GLU:OE1	2.17	0.43
1:I:90:ASN:ND2	1:I:137:ARG:O	2.52	0.43
1:D:66:ASN:C	1:D:66:ASN:HD22	2.26	0.43
1:A:66:ASN:C	1:A:66:ASN:HD22	2.26	0.43
1:C:29:VAL:O	1:C:152:VAL:HA	2.19	0.43
1:H:32:SER:HA	1:H:178:GLN:HE22	1.84	0.43
1:B:21:THR:HG23	1:B:23:ARG:O	2.19	0.43
1:F:159:SER:O	1:F:160:ASP:O	2.36	0.43
1:D:154:PRO:HG3	1:D:180:LYS:HB2	2.01	0.43
1:F:14:SER:HB3	3:F:2002:HOH:O	2.17	0.43
1:H:187:CYS:C	1:H:188:CYS:SG	3.02	0.42
1:J:155:THR:HG23	1:J:155:THR:O	2.19	0.42
1:C:145:HIS:CE1	1:D:75:SER:CB	3.02	0.42
1:A:146:HIS:HE1	1:A:148:ARG:HB2	1.84	0.42
1:B:29:VAL:O	1:B:152:VAL:HA	2.19	0.42
1:J:144:THR:HG22	2:J:1206:CCE:N6	2.34	0.42
1:I:152:VAL:O	1:I:180:LYS:HE3	2.20	0.42
1:C:66:ASN:C	1:C:66:ASN:HD22	2.27	0.42
1:I:29:VAL:O	1:I:152:VAL:HA	2.19	0.42
1:J:187:CYS:SG	1:J:188:CYS:N	2.93	0.42
1:F:124:ASP:HB2	1:G:168:TYR:CE1	2.55	0.42
1:H:44:ILE:HG22	1:I:170:ARG:HD3	2.02	0.41
1:G:179:LYS:NZ	1:G:196:GLU:OE1	2.54	0.41
1:J:143:TRP:O	2:J:1206:CCE:H2C2	2.20	0.41
1:B:70:SER:HB3	1:B:71:PRO:HD2	2.02	0.41
1:F:88:ALA:HA	1:F:139:LYS:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:HB2	1:B:168:TYR:CE1	2.55	0.41
1:J:66:ASN:HD22	1:J:68:SER:H	1.67	0.41
1:A:143:TRP:CE2	1:B:99:THR:HG21	2.56	0.41
1:C:145:HIS:HD2	1:C:150:ILE:HD11	1.85	0.41
1:F:50:VAL:HG12	1:F:52:PHE:HD1	1.86	0.41
1:I:143:TRP:CE2	1:J:99:THR:HG21	2.56	0.41
1:I:187:CYS:C	1:I:188:CYS:SG	3.04	0.41
1:F:112:LEU:HD23	2:J:1206:CCE:O7	2.19	0.41
1:B:3:ARG:HD3	3:B:2004:HOH:O	2.21	0.40
1:E:32:SER:HA	1:E:178:GLN:HE22	1.86	0.40
1:D:33:LEU:CD2	1:D:54:GLN:HG3	2.51	0.40
1:E:156:THR:C	1:E:158:ASN:H	2.28	0.40
1:G:125:VAL:O	1:G:125:VAL:HG12	2.21	0.40
1:H:90:ASN:ND2	1:H:137:ARG:O	2.55	0.40
1:D:183:VAL:HG11	1:D:185:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	203/210 (97%)	192 (95%)	11 (5%)	0	100	100
1	B	203/210 (97%)	199 (98%)	3 (2%)	1 (0%)	24	43
1	C	203/210 (97%)	196 (97%)	6 (3%)	1 (0%)	24	43
1	D	203/210 (97%)	200 (98%)	3 (2%)	0	100	100
1	E	203/210 (97%)	196 (97%)	7 (3%)	0	100	100
1	F	203/210 (97%)	193 (95%)	6 (3%)	4 (2%)	6	10
1	G	203/210 (97%)	195 (96%)	7 (3%)	1 (0%)	24	43
1	H	203/210 (97%)	194 (96%)	7 (3%)	2 (1%)	12	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	203/210 (97%)	198 (98%)	5 (2%)	0	100	100
1	J	203/210 (97%)	199 (98%)	3 (2%)	1 (0%)	24	43
All	All	2030/2100 (97%)	1962 (97%)	58 (3%)	10 (0%)	24	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	SER
1	F	160	ASP
1	H	159	SER
1	F	189	PRO
1	J	23	ARG
1	C	160	ASP
1	F	159	SER
1	F	156	THR
1	H	158	ASN
1	G	154	PRO

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	191/196 (97%)	175 (92%)	16 (8%)	10	22
1	B	191/196 (97%)	174 (91%)	17 (9%)	9	20
1	C	191/196 (97%)	174 (91%)	17 (9%)	9	20
1	D	191/196 (97%)	172 (90%)	19 (10%)	7	16
1	E	191/196 (97%)	175 (92%)	16 (8%)	10	22
1	F	191/196 (97%)	176 (92%)	15 (8%)	11	24
1	G	191/196 (97%)	175 (92%)	16 (8%)	10	22
1	H	191/196 (97%)	173 (91%)	18 (9%)	8	18
1	I	191/196 (97%)	172 (90%)	19 (10%)	7	16
1	J	191/196 (97%)	173 (91%)	18 (9%)	8	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1910/1960 (97%)	1739 (91%)	171 (9%)	9 19

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	23	ARG
1	A	32	SER
1	A	48	VAL
1	A	50	VAL
1	A	57	THR
1	A	59	SER
1	A	66	ASN
1	A	129	ASP
1	A	137	ARG
1	A	151	SER
1	A	157	GLU
1	A	179	LYS
1	A	186	SER
1	A	188	CYS
1	A	203	LYS
1	B	21	THR
1	B	22	GLN
1	B	23	ARG
1	B	30	SER
1	B	32	SER
1	B	48	VAL
1	B	50	VAL
1	B	57	THR
1	B	59	SER
1	B	66	ASN
1	B	68	SER
1	B	129	ASP
1	B	137	ARG
1	B	152	VAL
1	B	157	GLU
1	B	161	ASP
1	B	203	LYS
1	C	21	THR
1	C	23	ARG
1	C	32	SER
1	C	48	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	50	VAL
1	C	57	THR
1	C	59	SER
1	C	66	ASN
1	C	69	HIS
1	C	70	SER
1	C	129	ASP
1	C	137	ARG
1	C	156	THR
1	C	180	LYS
1	C	182	SER
1	C	188	CYS
1	C	203	LYS
1	D	15	ARG
1	D	21	THR
1	D	22	GLN
1	D	25	ARG
1	D	32	SER
1	D	48	VAL
1	D	50	VAL
1	D	57	THR
1	D	59	SER
1	D	66	ASN
1	D	68	SER
1	D	101	GLN
1	D	129	ASP
1	D	137	ARG
1	D	158	ASN
1	D	159	SER
1	D	160	ASP
1	D	164	TYR
1	D	203	LYS
1	E	21	THR
1	E	23	ARG
1	E	25	ARG
1	E	32	SER
1	E	48	VAL
1	E	50	VAL
1	E	57	THR
1	E	59	SER
1	E	66	ASN
1	E	129	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	137	ARG
1	E	139	LYS
1	E	151	SER
1	E	157	GLU
1	E	179	LYS
1	E	203	LYS
1	F	21	THR
1	F	32	SER
1	F	48	VAL
1	F	50	VAL
1	F	57	THR
1	F	59	SER
1	F	66	ASN
1	F	101	GLN
1	F	110	GLU
1	F	129	ASP
1	F	137	ARG
1	F	160	ASP
1	F	179	LYS
1	F	193	GLU
1	F	203	LYS
1	G	21	THR
1	G	24	ASP
1	G	25	ARG
1	G	32	SER
1	G	48	VAL
1	G	50	VAL
1	G	57	THR
1	G	59	SER
1	G	66	ASN
1	G	129	ASP
1	G	137	ARG
1	G	139	LYS
1	G	156	THR
1	G	161	ASP
1	G	182	SER
1	G	203	LYS
1	H	21	THR
1	H	32	SER
1	H	48	VAL
1	H	50	VAL
1	H	57	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	59	SER
1	H	66	ASN
1	H	112	LEU
1	H	129	ASP
1	H	137	ARG
1	H	155	THR
1	H	156	THR
1	H	158	ASN
1	H	163	GLU
1	H	180	LYS
1	H	186	SER
1	H	190	GLU
1	H	203	LYS
1	I	21	THR
1	I	25	ARG
1	I	32	SER
1	I	48	VAL
1	I	50	VAL
1	I	57	THR
1	I	59	SER
1	I	66	ASN
1	I	101	GLN
1	I	110	GLU
1	I	112	LEU
1	I	129	ASP
1	I	137	ARG
1	I	139	LYS
1	I	157	GLU
1	I	161	ASP
1	I	179	LYS
1	I	180	LYS
1	I	203	LYS
1	J	21	THR
1	J	23	ARG
1	J	25	ARG
1	J	32	SER
1	J	48	VAL
1	J	50	VAL
1	J	57	THR
1	J	59	SER
1	J	66	ASN
1	J	101	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	112	LEU
1	J	129	ASP
1	J	137	ARG
1	J	156	THR
1	J	159	SER
1	J	180	LYS
1	J	182	SER
1	J	203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	145	HIS
1	A	200	ASN
1	B	22	GLN
1	B	66	ASN
1	B	101	GLN
1	B	146	HIS
1	B	158	ASN
1	C	54	GLN
1	C	66	ASN
1	C	145	HIS
1	C	146	HIS
1	C	200	ASN
1	D	101	GLN
1	D	119	GLN
1	D	145	HIS
1	D	200	ASN
1	E	22	GLN
1	E	66	ASN
1	E	145	HIS
1	E	178	GLN
1	F	66	ASN
1	F	101	GLN
1	F	158	ASN
1	G	66	ASN
1	G	101	GLN
1	G	146	HIS
1	G	158	ASN
1	H	66	ASN
1	H	145	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	200	ASN
1	I	55	GLN
1	I	66	ASN
1	I	145	HIS
1	I	200	ASN
1	J	66	ASN
1	J	101	GLN
1	J	200	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](#)

3 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	CCE	J	1206	-	9,9,9	2.51	1 (11%)	11,12,12	3.47	2 (18%)
2	CCE	D	1206	-	9,9,9	2.60	1 (11%)	11,12,12	2.82	3 (27%)
2	CCE	C	1206	-	9,9,9	2.85	1 (11%)	11,12,12	3.19	3 (27%)

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	CCE	J	1206	-	-	3/7/7/7	-
2	CCE	D	1206	-	-	3/7/7/7	-
2	CCE	C	1206	-	-	3/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1206	CCE	O4-C5	8.41	1.47	1.35
2	D	1206	CCE	O4-C5	7.62	1.46	1.35
2	J	1206	CCE	O4-C5	7.28	1.46	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1206	CCE	O4-C5-O7	-8.26	115.47	123.08
2	C	1206	CCE	O4-C5-N6	7.92	120.96	111.11
2	J	1206	CCE	O4-C5-N6	7.84	120.86	111.11
2	D	1206	CCE	O4-C5-N6	7.23	120.11	111.11
2	C	1206	CCE	O4-C5-O7	-6.46	117.12	123.08
2	D	1206	CCE	O4-C5-O7	-5.08	118.40	123.08
2	D	1206	CCE	O7-C5-N6	-2.59	121.50	125.58
2	C	1206	CCE	O7-C5-N6	-2.32	121.92	125.58

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1206	CCE	O7-C5-O4-C3
2	C	1206	CCE	N6-C5-O4-C3
2	D	1206	CCE	O7-C5-O4-C3
2	D	1206	CCE	N6-C5-O4-C3
2	J	1206	CCE	O7-C5-O4-C3
2	J	1206	CCE	N6-C5-O4-C3
2	C	1206	CCE	C2-C3-O4-C5
2	D	1206	CCE	C2-C3-O4-C5
2	J	1206	CCE	C2-C3-O4-C5

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1206	CCE	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

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.