WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 4, 2023 – 03:33 pm GMT

PDB ID : 2BR8
Title : Crystal Structure of Acetylcholine-binding Protein (AChBP) from Aplysia californica in complex with an alpha-conotoxin PnIA variant
Authors : Celie, P.H.N.; Kasheverov, I.E.; Mordvintsev, D.Y.; Hogg, R.C.; van Nierop, P.; van Elk, R.; van Rossum-Fikkert, S.E.; Zhmak, M.N.; Bertrand, D.; Tsetlin, V.; Sixma, T.K.; Smit, A.B.
Deposited on : 2005-05-03
Resolution : 2.40 Å(reported)

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

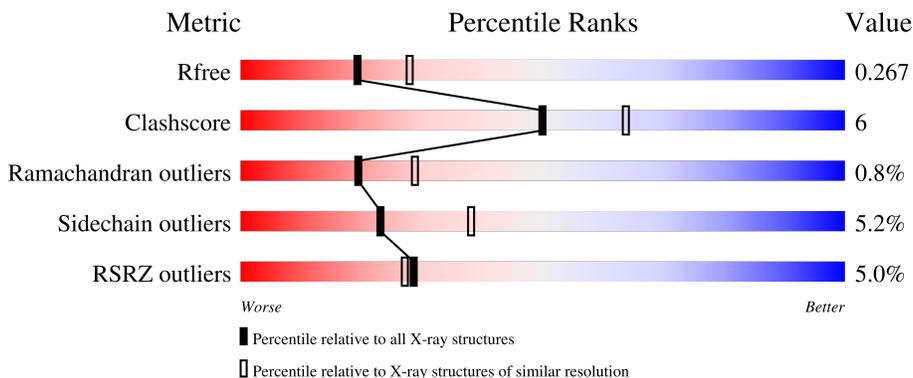|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 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 2.40 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.
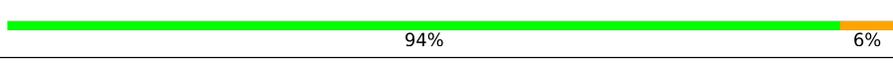
Metric	Percentile Ranks	Value
Rfree		0.267
Clashscore		6
Ramachandran outliers		0.8%
Sidechain outliers		5.2%
RSRZ outliers		5.0%

Worse ——— *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	217	6% / 76% 17% · 6%
1	B	217	6% / 77% 14% · 6%
1	C	217	4% / 75% 17% · 6%
1	D	217	.% / 76% 16% · 6%

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Mol	Chain	Length	Quality of chain
1	E	217	6% 84% 10% · 6%
2	F	17	6% 65% 35%
2	G	17	76% 18% 6%
2	H	17	94% 6%
2	I	17	76% 24%
2	J	17	12% 82% 18%
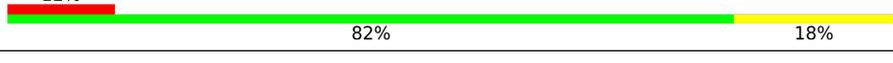
2 Entity composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9010 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	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	B	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	C	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	D	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			
1	E	205	Total	C	N	O	S	0	0	0
			1636	1036	266	325	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	VAL	ALA	conflict	UNP Q8WSF8
A	136	VAL	ALA	conflict	UNP Q8WSF8
B	41	VAL	ALA	conflict	UNP Q8WSF8
B	136	VAL	ALA	conflict	UNP Q8WSF8
C	41	VAL	ALA	conflict	UNP Q8WSF8
C	136	VAL	ALA	conflict	UNP Q8WSF8
D	41	VAL	ALA	conflict	UNP Q8WSF8
D	136	VAL	ALA	conflict	UNP Q8WSF8
E	41	VAL	ALA	conflict	UNP Q8WSF8
E	136	VAL	ALA	conflict	UNP Q8WSF8

- Molecule 2 is a protein called ALPHA-CONOTOXIN PNIA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	17	Total	C	N	O	S	0	0	1
			114	70	20	20	4			
2	G	17	Total	C	N	O	S	0	0	1
			114	70	20	20	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	17	Total	C	N	O	S	0	0	1
			114	70	20	20	4			
2	I	17	Total	C	N	O	S	0	0	1
			114	70	20	20	4			
2	J	17	Total	C	N	O	S	0	0	1
			114	70	20	20	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	10	LEU	ALA	engineered mutation	UNP P50984
F	14	LYS	ASP	engineered mutation	UNP P50984
G	10	LEU	ALA	engineered mutation	UNP P50984
G	14	LYS	ASP	engineered mutation	UNP P50984
H	10	LEU	ALA	engineered mutation	UNP P50984
H	14	LYS	ASP	engineered mutation	UNP P50984
I	10	LEU	ALA	engineered mutation	UNP P50984
I	14	LYS	ASP	engineered mutation	UNP P50984
J	10	LEU	ALA	engineered mutation	UNP P50984
J	14	LYS	ASP	engineered mutation	UNP P50984

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
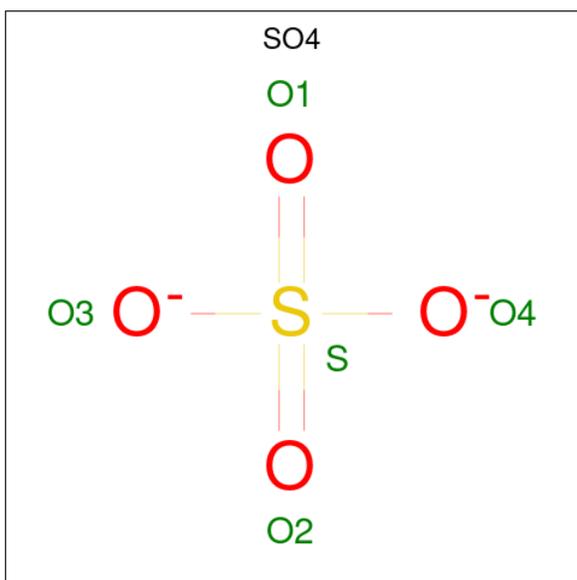
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	G	1	Total 5	O 4	S 1	0	0
3	I	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total 35	O 35	0	0
4	B	38	Total 38	O 38	0	0
4	C	71	Total 71	O 71	0	0
4	D	51	Total 51	O 51	0	0
4	E	26	Total 26	O 26	0	0
4	G	4	Total 4	O 4	0	0
4	H	5	Total 5	O 5	0	0
4	I	4	Total 4	O 4	0	0
4	J	1	Total 1	O 1	0	0

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 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.
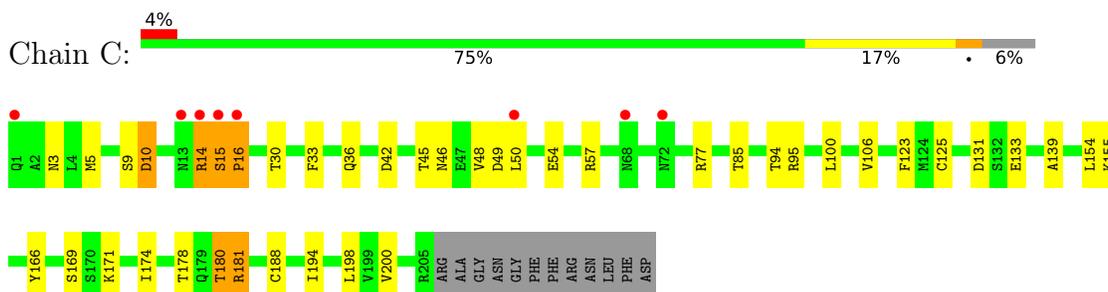
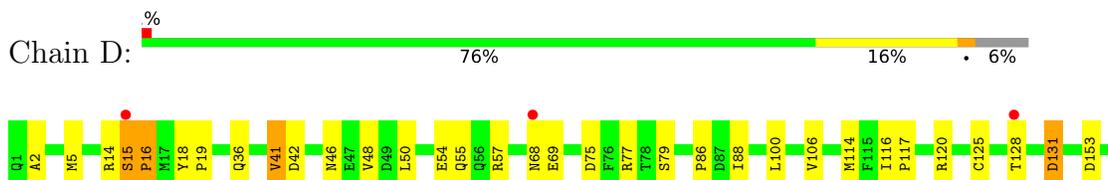- Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR
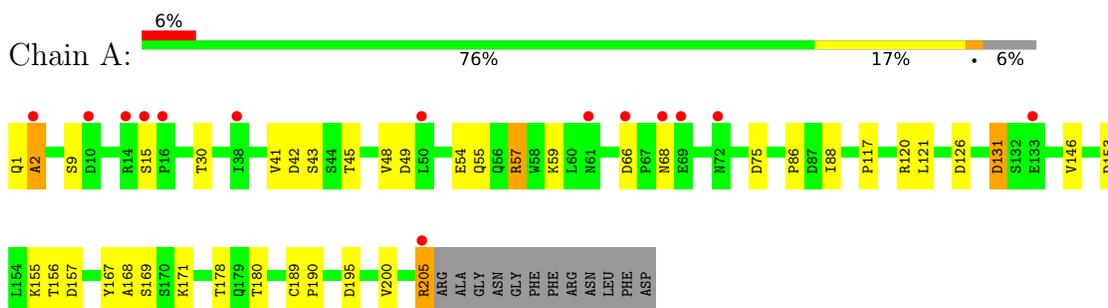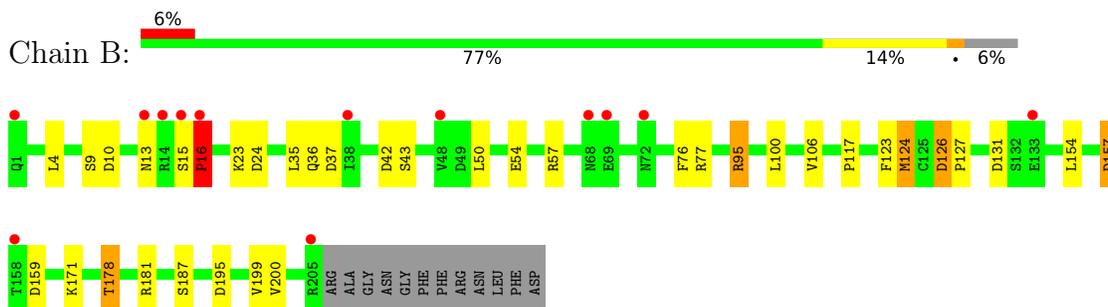
Chain A:

- Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain B:

- Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain C:

- Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain D:

S165 Y166 Y167 A168 S169 S170 K171 T178 R181 Y193 R205 ARG ALA GLY ASN GLY PHE PHE ARG ASN LEU PHE ASP

● Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR

Chain E:

6%
84%   10%   6%

Q1 M5 S9 D10 L11 F12 N13 R14 S15 P16 D25 D42 T45 N68 E69 N72 R77 T78 S79 D82 T94 V97 M114 F115 I116 G129 V130 D131 S132 E133 E134 V146 D153 T178 Q179 T180 Y186 S187 C188 C189 D195

R205 ARG ALA GLY ASN GLY PHE PHE ARG ASN LEU PHE ASP

● Molecule 2: ALPHA-CONOTOXIN PNIA

Chain F:

6%
65%   35%

G1 P6 P7 L10 N11 N12 P13 K14 NH217

● Molecule 2: ALPHA-CONOTOXIN PNIA

Chain G:

76%   18%   6%

G1 P7 L10 P13 NH217

● Molecule 2: ALPHA-CONOTOXIN PNIA

Chain H:

94%   6%

G1 L10 NH217

● Molecule 2: ALPHA-CONOTOXIN PNIA

Chain I:

76%   24%

G1 P6 P7 C8 A9 NH217

● Molecule 2: ALPHA-CONOTOXIN PNIA

Chain J:

12%
82%   18%

G1 P6 P7 L10 K14 Y15 C16 NH217
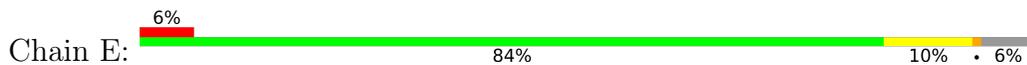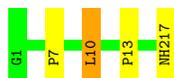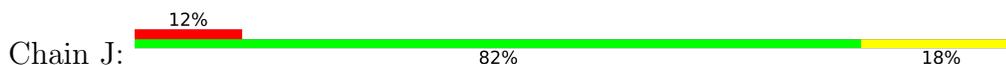
4 Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.47Å 80.08Å 134.04Å 90.00° 93.20° 90.00°	Depositor
Resolution (Å)	19.80 – 2.40 19.80 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.80-2.40) 97.8 (19.80-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.198 , 0.250 0.225 , 0.267	Depositor DCC
R_{free} test set	2783 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.8	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9010	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NH2

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	0.44	0/1676	0.80	5/2287 (0.2%)
1	B	0.49	0/1676	0.85	9/2287 (0.4%)
1	C	0.57	0/1676	0.88	3/2287 (0.1%)
1	D	0.49	0/1676	0.82	3/2287 (0.1%)
1	E	0.46	0/1676	0.82	5/2287 (0.2%)
2	F	0.49	0/116	0.75	0/158
2	G	0.51	0/116	0.65	0/158
2	H	0.58	0/116	0.65	0/158
2	I	0.45	0/116	0.61	0/158
2	J	0.42	0/116	0.60	0/158
All	All	0.49	0/8960	0.82	25/12225 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	131	ASP	CB-CG-OD2	6.49	124.14	118.30
1	E	153	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	195	ASP	CB-CG-OD2	6.22	123.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	131	ASP	CB-CG-OD2	6.17	123.86	118.30
1	B	131	ASP	CB-CG-OD2	6.05	123.74	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	16	PRO	Peptide
1	C	16	PRO	Peptide
1	C	188	CYS	Peptide
1	D	15	SER	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	1572	23	0
1	B	1636	0	1572	26	0
1	C	1636	0	1572	22	0
1	D	1636	0	1572	21	0
1	E	1636	0	1572	11	0
2	F	114	0	108	4	0
2	G	114	0	108	2	0
2	H	114	0	108	1	0
2	I	114	0	108	4	0
2	J	114	0	108	2	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	I	5	0	0	0	0
4	A	35	0	0	1	0
4	B	38	0	0	4	0
4	C	71	0	0	4	0
4	D	51	0	0	4	0
4	E	26	0	0	0	0
4	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	5	0	0	0	0
4	I	4	0	0	0	0
4	J	1	0	0	0	0
All	All	9010	0	8400	99	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 6.

The worst 5 of 99 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:B:95:ARG:HG2	1:B:95:ARG:HH11	1.38	0.87
1:B:50:LEU:HB3	4:B:2008:HOH:O	1.73	0.86
1:B:154:LEU:O	1:B:181:ARG:HD2	1.76	0.85
1:D:16:PRO:HD3	4:D:2004:HOH:O	1.77	0.82
1:A:57:ARG:HH11	1:A:57:ARG:HG3	1.44	0.82

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	203/217 (94%)	198 (98%)	3 (2%)	2 (1%)	15	23
1	B	203/217 (94%)	192 (95%)	10 (5%)	1 (0%)	29	41
1	C	203/217 (94%)	192 (95%)	9 (4%)	2 (1%)	15	23
1	D	203/217 (94%)	194 (96%)	6 (3%)	3 (2%)	10	14
1	E	203/217 (94%)	195 (96%)	7 (3%)	1 (0%)	29	41
2	F	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
2	G	15/17 (88%)	15 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	15/17 (88%)	15 (100%)	0	0	100	100
2	I	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
2	J	15/17 (88%)	15 (100%)	0	0	100	100
All	All	1090/1170 (93%)	1044 (96%)	37 (3%)	9 (1%)	19	29

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	C	15	SER
1	D	15	SER
1	E	15	SER
1	B	16	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	188/197 (95%)	180 (96%)	8 (4%)	29	46
1	B	188/197 (95%)	178 (95%)	10 (5%)	22	37
1	C	188/197 (95%)	176 (94%)	12 (6%)	17	28
1	D	188/197 (95%)	174 (93%)	14 (7%)	13	22
1	E	188/197 (95%)	182 (97%)	6 (3%)	39	59
2	F	14/14 (100%)	14 (100%)	0	100	100
2	G	14/14 (100%)	12 (86%)	2 (14%)	3	4
2	H	14/14 (100%)	13 (93%)	1 (7%)	14	23
2	I	14/14 (100%)	14 (100%)	0	100	100
2	J	14/14 (100%)	14 (100%)	0	100	100
All	All	1010/1055 (96%)	957 (95%)	53 (5%)	23	38

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	194	ILE
1	D	77	ARG
1	E	180	THR
1	C	200	VAL
1	D	41	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	55	GLN
1	D	119	GLN
1	D	72	ASN
1	D	184	GLN
1	B	72	ASN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5　Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6　Ligand geometry ⓘ

5 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	$\#|Z| > 2$
3	SO4	C	1206	-	4,4,4	0.17	0	6,6,6	0.27	0
3	SO4	F	1018	-	4,4,4	0.12	0	6,6,6	0.13	0
3	SO4	G	1018	-	4,4,4	0.19	0	6,6,6	0.11	0
3	SO4	E	1206	-	4,4,4	0.12	0	6,6,6	0.10	0
3	SO4	I	1018	-	4,4,4	0.13	0	6,6,6	0.28	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	J	1
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	16:CYS	C	17:NH2	N	1.65
1	H	16:CYS	C	17:NH2	N	1.04

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(Å²)	Q<0.9
1	A	205/217 (94%)	0.19	14 (6%)	17	15	18, 25, 41, 52	0
1	B	205/217 (94%)	0.11	13 (6%)	20	18	11, 19, 48, 56	0
1	C	205/217 (94%)	0.20	8 (3%)	39	38	10, 21, 47, 60	0
1	D	205/217 (94%)	-0.27	3 (1%)	73	72	7, 15, 24, 38	0
1	E	205/217 (94%)	-0.01	14 (6%)	17	15	10, 17, 37, 44	0
2	F	16/17 (94%)	0.46	1 (6%)	20	18	21, 23, 27, 27	0
2	G	16/17 (94%)	-0.05	0	100	100	19, 22, 24, 25	0
2	H	16/17 (94%)	0.06	0	100	100	13, 17, 19, 20	0
2	I	16/17 (94%)	0.04	0	100	100	23, 25, 27, 27	0
2	J	16/17 (94%)	0.46	2 (12%)	3	3	31, 33, 35, 35	0
All	All	1105/1170 (94%)	0.05	55 (4%)	28	27	7, 20, 40, 60	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	PRO	7.1
1	E	15	SER	5.4
1	B	15	SER	5.4
1	C	15	SER	5.3
1	B	68	ASN	4.5

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 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
3	SO4	E	1206	5/5	0.80	0.27	90,91,91,91	0
3	SO4	F	1018	5/5	0.88	0.19	76,76,76,77	0
3	SO4	G	1018	5/5	0.98	0.19	38,38,40,40	0
3	SO4	I	1018	5/5	0.98	0.12	27,27,28,28	0
3	SO4	C	1206	5/5	0.99	0.11	18,19,20,20	0

6.5   Other polymers (i)

There are no such residues in this entry.