



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:05 pm GMT

PDB ID : 2BYQ  
Title : CRYSTAL STRUCTURE OF APLYSIA CALIFORNICA ACHBP IN COM-  
PLEX WITH EPIBATIDINE  
Authors : Hansen, S.B.; Sulzenbacher, G.; Huxford, T.; Marchot, P.; Taylor, P.; Bourne,  
Y.  
Deposited on : 2005-08-03  
Resolution : 3.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

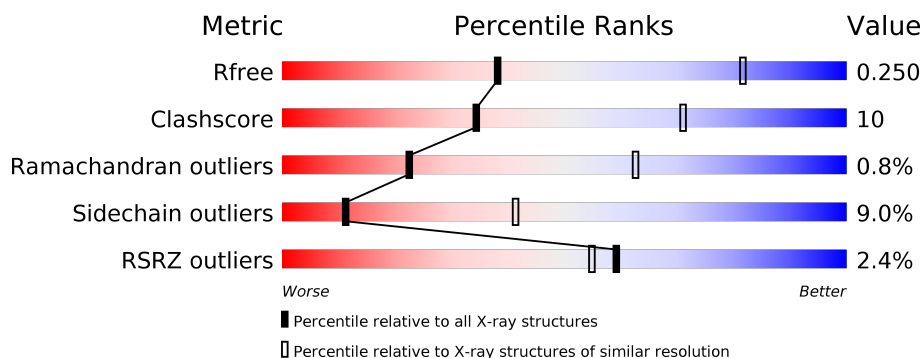
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	227	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>• 6%</div> </div> </div>
1	B	227	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>• 6%</div> </div> </div>
1	C	227	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>23%</div> <div>• 6%</div> </div> </div>
1	D	227	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>26%</div> <div>• 6%</div> </div> </div>
1	E	227	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• 6%</div> </div> </div>

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
2	EPJ	B	300	-	-	X	-

## 2 Entry composition [i](#)

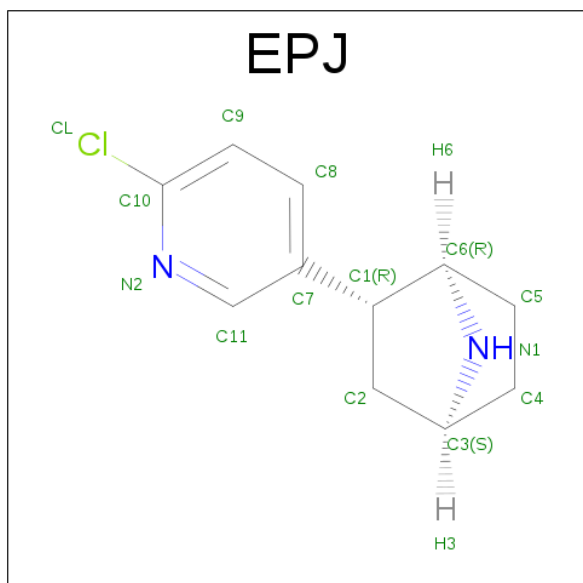
There are 2 unique types of molecules in this entry. The entry contains 8585 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	4	0
			1706	1075	281	341	9			
1	B	214	Total	C	N	O	S	0	2	0
			1700	1070	281	341	8			
1	C	214	Total	C	N	O	S	0	1	0
			1703	1072	281	341	9			
1	D	214	Total	C	N	O	S	0	1	0
			1706	1075	281	341	9			
1	E	213	Total	C	N	O	S	0	0	0
			1700	1071	280	340	9			

- Molecule 2 is EPIBATIDINE (three-letter code: EPJ) (formula:  $C_{11}H_{13}ClN_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			14	11	1	2		

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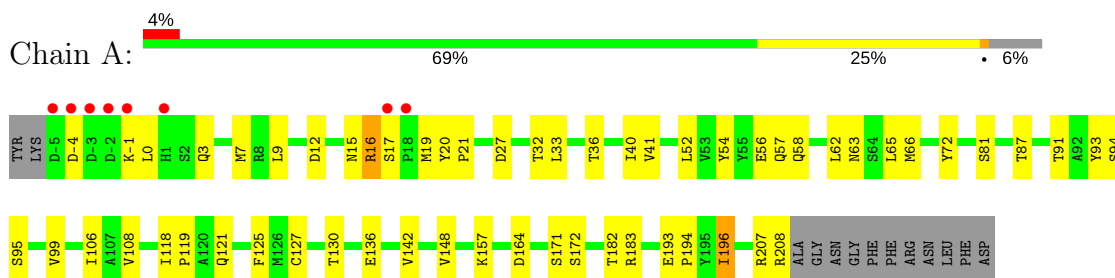
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	0	0
			14	11	1	2		
2	C	1	Total	C	Cl	N	0	0
			14	11	1	2		
2	D	1	Total	C	Cl	N	0	0
			14	11	1	2		
2	E	1	Total	C	Cl	N	0	0
			14	11	1	2		

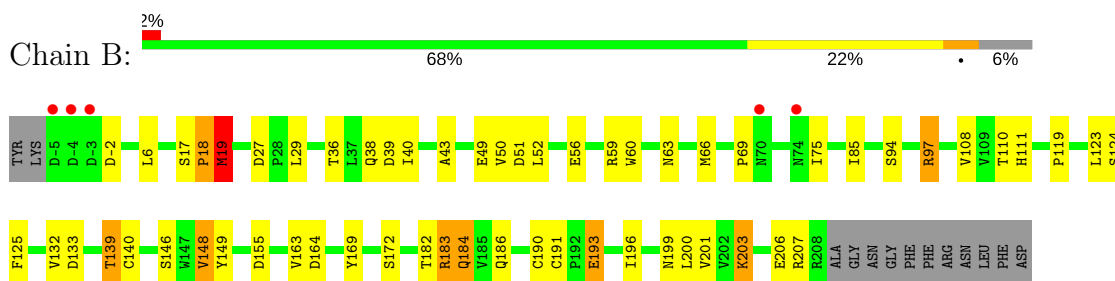
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

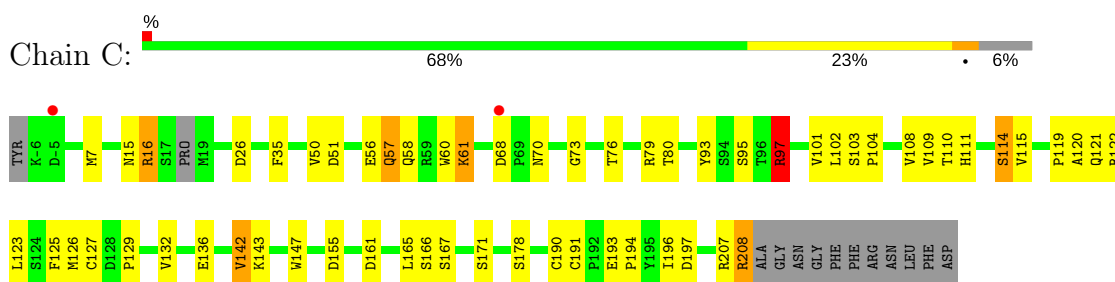
#### • Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



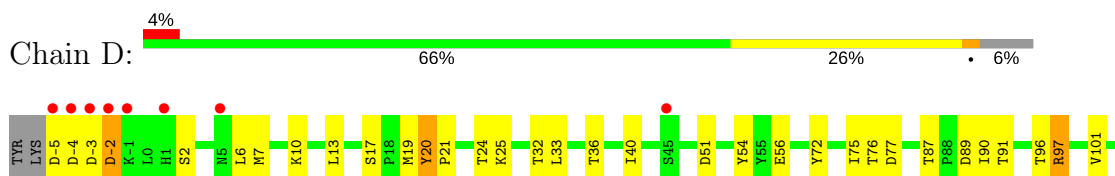
#### • Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



#### • Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR



#### • Molecule 1: SOLUBLE ACETYLCHOLINE RECEPTOR





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.93Å 200.93Å 200.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.40 29.62 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-3.40) 96.8 (29.62-3.40)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 3.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.180 , 0.255 0.185 , 0.250	Depositor DCC
$R_{free}$ test set	929 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 30.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.039 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EPJ

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	0.55	0/1747	0.69	0/2381
1	B	0.58	1/1740 (0.1%)	0.73	1/2372 (0.0%)
1	C	0.59	0/1742	0.74	1/2372 (0.0%)
1	D	0.57	0/1747	0.71	0/2381
1	E	0.55	0/1741	0.71	0/2373
All	All	0.57	1/8717 (0.0%)	0.72	2/11879 (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	B	0	1
1	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	CYS	CB-SG	-5.14	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	PRO	N-CA-CB	7.19	111.93	103.30
1	C	97	ARG	NE-CZ-NH1	5.88	123.24	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	19	MET	Peptide
1	E	19	MET	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	1706	0	1629	30	0
1	B	1700	0	1612	37	0
1	C	1703	0	1621	40	0
1	D	1706	0	1629	37	0
1	E	1700	0	1625	31	0
2	A	14	0	13	2	0
2	B	14	0	13	6	0
2	C	14	0	13	3	0
2	D	14	0	13	2	0
2	E	14	0	13	4	0
All	All	8585	0	8181	160	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 10.

All (160) 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:C:97:ARG:HH11	1:C:97:ARG:HG3	1.35	0.91
1:D:139:THR:HG23	1:D:203:LYS:HG2	1.59	0.85
1:C:193:GLU:HB3	1:C:194:PRO:HD2	1.58	0.84
1:D:97:ARG:HG3	1:D:124:SER:HB2	1.64	0.80
1:D:36:THR:HA	1:D:164:ASP:HB3	1.63	0.79
1:A:93:TYR:HE1	2:A:300:EPJ:H4C1	1.55	0.72
1:A:148:VAL:HG21	1:E:106:ILE:HB	1.74	0.70
1:A:172:SER:O	1:A:207:ARG:NH1	2.27	0.68
1:B:193:GLU:H	1:B:193:GLU:CD	1.98	0.68
1:C:95:SER:HB3	1:C:123:LEU:HD11	1.76	0.67
1:B:40:ILE:HG12	1:B:52:LEU:HD23	1.77	0.67
1:D:-5:ASP:HB3	1:D:-2:ASP:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ARG:HG3	1:C:97:ARG:NH1	2.04	0.64
1:D:106:ILE:HB	1:E:148:VAL:HG11	1.78	0.64
1:A:40:ILE:HG12	1:A:52:LEU:CD2	2.29	0.63
1:A:125:PHE:CD1	1:A:142:VAL:HB	2.33	0.62
1:E:71:GLU:HB2	1:E:72:TYR:CD2	2.34	0.62
1:E:55:TYR:HB3	1:E:120:ALA:HA	1.80	0.61
1:C:122:ARG:HD2	1:D:96:THR:O	1.99	0.61
1:B:163:VAL:HG21	1:B:200:LEU:HD13	1.83	0.61
1:B:52:LEU:HD11	1:B:125:PHE:CE2	2.35	0.60
1:B:110:THR:HG22	1:B:111:HIS:CD2	2.36	0.60
1:A:183:ARG:HH21	1:A:196:ILE:HD12	1.66	0.60
1:A:93:TYR:CE1	2:A:300:EPJ:H4C1	2.36	0.59
1:B:36:THR:HA	1:B:164:ASP:HB3	1.84	0.59
1:A:41:VAL:CG1	1:B:49:GLU:OE1	2.51	0.58
1:A:118:ILE:HB	2:B:300:EPJ:H8	1.85	0.58
1:D:72:TYR:O	1:D:75:ILE:HG13	2.04	0.58
1:E:-1:LYS:O	1:E:3:GLN:HG2	2.04	0.58
1:D:33:LEU:HD11	1:D:90:ILE:HD12	1.85	0.57
1:D:97:ARG:HG3	1:D:124:SER:CB	2.34	0.57
1:A:207:ARG:O	1:A:208:ARG:HB2	2.05	0.57
1:B:163:VAL:HG21	1:B:200:LEU:CD1	2.35	0.57
1:C:104:PRO:HG2	1:D:89:ASP:HB2	1.86	0.56
1:E:147:TRP:O	2:E:300:EPJ:H2C1	2.05	0.56
1:B:97:ARG:HG3	1:B:124:SER:HB2	1.87	0.56
1:B:39:ASP:OD1	1:B:172:SER:HB2	2.05	0.56
1:B:148:VAL:HG12	2:B:300:EPJ:C10	2.35	0.56
1:A:-4:ASP:OD1	1:A:-1:LYS:HD2	2.06	0.56
1:C:50:VAL:HG21	1:C:127:CYS:SG	2.45	0.56
1:E:40:ILE:HD11	1:E:176:ILE:CD1	2.36	0.56
1:B:172:SER:O	1:B:207:ARG:NH1	2.39	0.55
1:C:108:VAL:HG23	2:D:300:EPJ:CL	2.44	0.55
1:B:148:VAL:HG12	2:B:300:EPJ:CL	2.44	0.55
1:C:7:MET:HG3	1:D:21:PRO:HG3	1.89	0.54
1:B:190:CYS:SG	2:B:300:EPJ:H2C2	2.49	0.52
1:D:7:MET:HE2	1:E:20:TYR:HA	1.90	0.52
1:B:169:TYR:CD2	1:C:126:MET:HB3	2.44	0.51
1:A:36:THR:HA	1:A:164:ASP:HB3	1.92	0.51
1:A:62:LEU:HD12	1:A:65:LEU:HD12	1.92	0.51
1:D:6:LEU:O	1:D:10:LYS:HG3	2.11	0.51
1:B:110:THR:HG22	1:B:111:HIS:HD2	1.76	0.50
1:B:108:VAL:HG23	2:C:300:EPJ:CL	2.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:TYR:CZ	1:D:121:GLN:HG3	2.47	0.50
1:C:109:VAL:HG22	1:C:115:VAL:HG22	1.92	0.50
1:D:13:LEU:O	1:D:17:SER:HB2	2.12	0.50
1:A:193[A]:GLU:HB3	1:A:194:PRO:HD2	1.94	0.49
1:E:125:PHE:CD1	1:E:142:VAL:HB	2.46	0.49
1:C:35:PHE:CE1	1:C:56:GLU:HG3	2.47	0.49
1:E:60:TRP:CH2	1:E:88:PRO:HD3	2.47	0.49
1:C:61:LYS:HG3	1:C:114:SER:HB3	1.95	0.49
1:D:77:ASP:HB3	1:D:110:THR:HG23	1.93	0.49
1:E:71:GLU:HB2	1:E:72:TYR:CE2	2.47	0.49
1:A:7:MET:SD	1:B:19:MET:HA	2.53	0.48
1:B:146:SER:OG	1:B:149:TYR:HB2	2.13	0.48
1:E:96:THR:O	1:E:97:ARG:HG3	2.13	0.48
1:C:110:THR:HG22	1:C:111:HIS:CD2	2.49	0.47
1:D:108:VAL:HG22	2:E:300:EPJ:CL	2.50	0.47
1:A:63:ASN:HA	1:A:66:MET:HG3	1.97	0.47
1:B:193:GLU:N	1:B:193:GLU:CD	2.67	0.47
1:E:190:CYS:SG	2:E:300:EPJ:H1	2.54	0.47
1:C:136:GLU:CD	1:C:136:GLU:H	2.17	0.47
1:E:188:TYR:CD1	2:E:300:EPJ:H4C2	2.49	0.47
1:A:57:GLN:HG3	1:A:118:ILE:HG12	1.97	0.47
1:D:185:VAL:HG22	1:D:196:ILE:HD12	1.97	0.47
1:D:40:ILE:HD11	1:D:202:VAL:HG11	1.96	0.47
1:B:183:ARG:HG2	1:B:184:GLN:N	2.30	0.47
1:A:3:GLN:NE2	1:B:27:ASP:OD2	2.48	0.47
1:D:56:GLU:O	1:D:119:PRO:HD2	2.15	0.46
1:C:190:CYS:SG	1:C:191:CYS:N	2.89	0.46
1:B:38:GLN:NE2	1:C:93:TYR:O	2.48	0.46
1:D:152:PHE:HE2	1:D:193:GLU:HB2	1.80	0.46
1:E:63:ASN:O	1:E:66:MET:HB2	2.16	0.46
1:A:54:TYR:OH	1:A:121:GLN:NE2	2.48	0.46
1:C:58:GLN:HB3	1:C:60:TRP:HZ3	1.80	0.46
1:C:104:PRO:HD3	1:D:91:THR:OG1	2.15	0.46
1:C:93:TYR:HE2	2:C:300:EPJ:H4C1	1.80	0.46
1:C:110:THR:HG22	1:C:111:HIS:N	2.30	0.46
1:C:56:GLU:O	1:C:119:PRO:HD2	2.16	0.46
1:D:152:PHE:CE2	1:D:193:GLU:HB2	2.51	0.46
1:D:132:VAL:O	1:D:132:VAL:HG22	2.16	0.46
1:A:56:GLU:O	1:A:119:PRO:HD2	2.16	0.46
1:C:102:LEU:HD12	1:C:121:GLN:C	2.36	0.46
1:E:40:ILE:HD11	1:E:176:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:THR:HG22	1:C:111:HIS:H	1.80	0.46
1:E:32:THR:HA	1:E:157:LYS:O	2.15	0.46
2:B:300:EPJ:H11	2:B:300:EPJ:H2C1	1.74	0.45
1:D:51:ASP:HA	1:D:123:LEU:O	2.16	0.45
1:A:108:VAL:HG23	2:B:300:EPJ:CL	2.53	0.45
1:B:56:GLU:O	1:B:119:PRO:HD2	2.16	0.45
1:A:106:ILE:HB	1:B:148:VAL:HG21	1.98	0.45
1:A:12:ASP:O	1:A:16:ARG:HB2	2.16	0.45
1:C:193:GLU:CB	1:C:194:PRO:HD2	2.40	0.45
1:D:169:TYR:CD2	1:E:126:MET:HB3	2.52	0.45
1:B:63:ASN:O	1:B:66:MET:HB2	2.16	0.45
1:D:107:ALA:HB2	1:D:117:PHE:CD1	2.52	0.44
1:B:139:THR:HG23	1:B:203:LYS:HG3	2.00	0.44
1:E:40:ILE:CD1	1:E:176:ILE:HD11	2.48	0.44
1:C:125:PHE:CD1	1:C:142:VAL:HB	2.52	0.44
1:E:193:GLU:HB3	1:E:194:PRO:HD2	1.99	0.44
1:D:191:CYS:SG	2:D:300:EPJ:H8	2.58	0.44
1:B:155:ASP:OD1	1:B:183:ARG:NH2	2.51	0.43
1:B:43:ALA:HA	1:B:50:VAL:HG22	1.99	0.43
1:A:41:VAL:HG12	1:B:49:GLU:OE1	2.16	0.43
1:D:185:VAL:HG13	1:D:194:PRO:HB2	2.00	0.43
1:C:147:TRP:CE2	2:C:300:EPJ:H6	2.54	0.43
1:E:89:ASP:CG	1:E:89:ASP:O	2.56	0.43
1:E:10:LYS:HE3	1:E:14:PHE:HE1	1.83	0.43
1:C:50:VAL:CG2	1:C:127:CYS:SG	3.06	0.43
1:C:193:GLU:HB3	1:C:194:PRO:CD	2.38	0.43
1:C:155:ASP:HA	1:C:196:ILE:HD12	2.00	0.43
1:E:8:ARG:HG2	1:E:72:TYR:HE1	1.84	0.43
1:C:57:GLN:HE21	1:C:57:GLN:HB2	1.49	0.42
1:E:3:GLN:HE21	1:E:3:GLN:HB3	1.56	0.42
1:E:50:VAL:CG1	1:E:51:ASP:N	2.82	0.42
1:A:136:GLU:N	1:A:136:GLU:OE2	2.47	0.42
1:C:97:ARG:NH1	1:C:97:ARG:CG	2.80	0.42
1:A:32:THR:HA	1:A:157:LYS:O	2.19	0.42
1:C:16:ARG:HB2	1:C:16:ARG:HH11	1.85	0.42
1:E:79:ARG:N	1:E:79:ARG:HD2	2.34	0.42
1:A:9:LEU:HB2	1:A:72:TYR:CD1	2.55	0.42
1:C:129:PRO:O	1:C:132:VAL:HB	2.20	0.42
1:C:103:SER:HB3	1:C:120:ALA:HB3	2.02	0.41
1:D:20:TYR:HA	1:D:21:PRO:HD3	1.79	0.41
1:B:133:ASP:HB3	1:B:206:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:VAL:HG22	1:D:196:ILE:CD1	2.51	0.41
1:A:27:ASP:OD2	1:E:3:GLN:NE2	2.54	0.41
1:C:68:ASP:O	1:C:70:ASN:N	2.54	0.41
1:B:69:PRO:HB3	1:B:75:ILE:O	2.21	0.41
1:C:79:ARG:HG3	1:C:108:VAL:HG22	2.02	0.41
1:A:20:TYR:HA	1:A:21:PRO:HD3	1.75	0.41
1:A:33:LEU:CD2	1:A:58:GLN:HG2	2.50	0.41
1:E:40:ILE:HD11	1:E:176:ILE:HD12	2.02	0.41
1:B:29:LEU:HD11	1:B:60:TRP:HB2	2.03	0.41
1:D:150:SER:OG	1:D:193:GLU:HG3	2.20	0.41
1:D:161[A]:ASP:HA	1:D:181:GLN:HG3	2.03	0.41
1:E:57:GLN:HG3	1:E:118:ILE:HG12	2.02	0.41
1:E:187:HIS:HE1	1:E:194:PRO:HB3	1.85	0.41
1:B:51:ASP:HA	1:B:123:LEU:O	2.21	0.41
1:C:136:GLU:OE2	1:C:136:GLU:N	2.51	0.41
1:C:207:ARG:O	1:C:208:ARG:C	2.59	0.41
1:E:30:THR:HA	1:E:155:ASP:O	2.21	0.41
1:D:135:GLU:O	1:D:205:ARG:HD3	2.21	0.41
1:D:89:ASP:OD2	1:D:148:VAL:HG22	2.21	0.41
1:C:61:LYS:HA	1:C:114:SER:HA	2.03	0.40
1:B:184:GLN:HE22	1:B:199:ASN:HB2	1.85	0.40
1:B:184:GLN:NE2	1:B:199:ASN:HB2	2.37	0.40
1:D:110:THR:HG22	1:D:111:HIS:H	1.87	0.40
1:B:190:CYS:SG	1:B:191:CYS:N	2.93	0.40
1:D:25:LYS:HG3	1:D:152:PHE:HB3	2.02	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	212/227 (93%)	205 (97%)	6 (3%)	1 (0%)	32 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	212/227 (93%)	200 (94%)	9 (4%)	3 (1%)	13	51
1	C	210/227 (92%)	195 (93%)	13 (6%)	2 (1%)	18	59
1	D	212/227 (93%)	196 (92%)	14 (7%)	2 (1%)	20	61
1	E	211/227 (93%)	202 (96%)	9 (4%)	0	100	100
All	All	1057/1135 (93%)	998 (94%)	51 (5%)	8 (1%)	22	62

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	SER
1	B	18	PRO
1	B	19	MET
1	D	20	TYR
1	C	73	GLY
1	D	19	MET
1	A	19	MET
1	C	15	ASN

### 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	194/205 (95%)	179 (92%)	15 (8%)	15	49
1	B	192/205 (94%)	175 (91%)	17 (9%)	11	42
1	C	193/205 (94%)	173 (90%)	20 (10%)	8	34
1	D	194/205 (95%)	178 (92%)	16 (8%)	13	47
1	E	194/205 (95%)	175 (90%)	19 (10%)	9	37
All	All	967/1025 (94%)	880 (91%)	87 (9%)	11	41

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	LEU
1	A	15	ASN
1	A	16	ARG
1	A	17	SER
1	A	81	SER
1	A	87	THR
1	A	91	THR
1	A	94	SER
1	A	95	SER
1	A	99	VAL
1	A	127	CYS
1	A	130	THR
1	A	171	SER
1	A	182	THR
1	A	196	ILE
1	B	-2	ASP
1	B	6	LEU
1	B	59	ARG
1	B	85	ILE
1	B	94	SER
1	B	97	ARG
1	B	132	VAL
1	B	139	THR
1	B	148	VAL
1	B	182	THR
1	B	183	ARG
1	B	184	GLN
1	B	186	GLN
1	B	193	GLU
1	B	196	ILE
1	B	201	VAL
1	B	203	LYS
1	C	16	ARG
1	C	26	ASP
1	C	51	ASP
1	C	57	GLN
1	C	61	LYS
1	C	76	THR
1	C	80	THR
1	C	97	ARG
1	C	101	VAL
1	C	114	SER
1	C	142	VAL

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Mol	Chain	Res	Type
1	C	143	LYS
1	C	161	ASP
1	C	165	LEU
1	C	166	SER
1	C	167	SER
1	C	171	SER
1	C	178	SER
1	C	197	ASP
1	C	208	ARG
1	D	-4	ASP
1	D	-3	ASP
1	D	-2	ASP
1	D	2	SER
1	D	24	THR
1	D	32	THR
1	D	76	THR
1	D	87	THR
1	D	97	ARG
1	D	101	VAL
1	D	108	VAL
1	D	110	THR
1	D	143	LYS
1	D	182	THR
1	D	189	SER
1	D	208	ARG
1	E	1	HIS
1	E	3	GLN
1	E	19	MET
1	E	20	TYR
1	E	31	VAL
1	E	45	SER
1	E	87	THR
1	E	94	SER
1	E	99	VAL
1	E	124	SER
1	E	127	CYS
1	E	130	THR
1	E	157	LYS
1	E	161	ASP
1	E	171	SER
1	E	182	THR
1	E	185	VAL

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Mol	Chain	Res	Type
1	E	186	GLN
1	E	196	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	121	GLN
1	A	184	GLN
1	B	3	GLN
1	B	74	ASN
1	B	105	GLN
1	B	111	HIS
1	B	162	GLN
1	B	184	GLN
1	B	186	GLN
1	C	57	GLN
1	C	111	HIS
1	C	162	GLN
1	C	184	GLN
1	C	199	ASN
1	D	3	GLN
1	D	57	GLN
1	D	70	ASN
1	D	111	HIS
1	D	184	GLN
1	E	3	GLN
1	E	63	ASN
1	E	184	GLN
1	E	186	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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$
2	EPJ	A	300	-	16,16,16	1.32	3 (18%)	20,23,23	1.81	4 (20%)
2	EPJ	B	300	-	16,16,16	1.47	3 (18%)	20,23,23	1.96	5 (25%)
2	EPJ	C	300	-	16,16,16	1.78	4 (25%)	20,23,23	1.99	8 (40%)
2	EPJ	D	300	-	16,16,16	1.63	3 (18%)	20,23,23	2.06	7 (35%)
2	EPJ	E	300	-	16,16,16	1.42	3 (18%)	20,23,23	2.19	9 (45%)

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	EPJ	A	300	-	-	0/4/21/21	0/1/3/3
2	EPJ	B	300	-	-	0/4/21/21	0/1/3/3
2	EPJ	C	300	-	-	0/4/21/21	0/1/3/3
2	EPJ	D	300	-	-	0/4/21/21	0/1/3/3
2	EPJ	E	300	-	-	0/4/21/21	0/1/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	300	EPJ	C6-N1	-3.86	1.42	1.48
2	C	300	EPJ	C6-N1	-3.83	1.42	1.48
2	B	300	EPJ	C6-N1	-3.26	1.43	1.48
2	E	300	EPJ	C6-N1	-3.09	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	EPJ	C7-C1	-2.77	1.47	1.51
2	A	300	EPJ	C6-N1	-2.61	1.44	1.48
2	B	300	EPJ	C3-N1	-2.60	1.42	1.49
2	D	300	EPJ	C3-N1	-2.43	1.43	1.49
2	E	300	EPJ	C3-N1	-2.41	1.43	1.49
2	A	300	EPJ	C3-N1	-2.36	1.43	1.49
2	D	300	EPJ	C7-C1	-2.22	1.48	1.51
2	C	300	EPJ	C3-N1	-2.21	1.43	1.49
2	A	300	EPJ	C10-CL	2.26	1.78	1.74
2	B	300	EPJ	C10-CL	2.35	1.78	1.74
2	E	300	EPJ	C10-CL	2.43	1.78	1.74
2	C	300	EPJ	C10-CL	3.72	1.80	1.74

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	300	EPJ	C5-C6-C1	-4.95	104.58	109.74
2	A	300	EPJ	C2-C3-C4	-4.82	104.74	109.61
2	E	300	EPJ	C2-C3-C4	-4.49	105.08	109.61
2	B	300	EPJ	C7-C11-N2	-4.16	118.97	124.68
2	D	300	EPJ	C5-C6-C1	-4.04	105.53	109.74
2	D	300	EPJ	C7-C11-N2	-3.07	120.46	124.68
2	C	300	EPJ	C5-C6-C1	-3.01	106.60	109.74
2	C	300	EPJ	C7-C11-N2	-3.01	120.55	124.68
2	C	300	EPJ	C9-C10-N2	-2.83	120.58	124.81
2	B	300	EPJ	C4-C5-C6	-2.72	99.65	103.69
2	E	300	EPJ	C7-C11-N2	-2.66	121.02	124.68
2	B	300	EPJ	C2-C3-N1	-2.56	99.44	103.14
2	A	300	EPJ	C7-C11-N2	-2.56	121.16	124.68
2	D	300	EPJ	C8-C7-C1	-2.54	116.15	121.07
2	B	300	EPJ	C1-C6-N1	-2.53	97.88	102.38
2	A	300	EPJ	C2-C3-N1	-2.41	99.66	103.14
2	C	300	EPJ	C9-C8-C7	-2.34	118.83	121.20
2	E	300	EPJ	C9-C10-N2	-2.20	121.52	124.81
2	E	300	EPJ	C8-C7-C1	-2.12	116.97	121.07
2	E	300	EPJ	C9-C8-C7	-2.04	119.12	121.20
2	D	300	EPJ	C8-C7-C11	2.12	118.98	116.83
2	C	300	EPJ	C8-C9-C10	2.17	119.69	117.44
2	E	300	EPJ	C8-C7-C11	2.30	119.16	116.83
2	E	300	EPJ	CL-C10-N2	2.38	121.04	116.10
2	D	300	EPJ	C11-N2-C10	2.53	119.62	116.37
2	E	300	EPJ	C11-N2-C10	2.60	119.72	116.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	300	EPJ	C2-C1-C6	2.63	105.55	102.38
2	C	300	EPJ	CL-C10-N2	2.73	121.78	116.10
2	A	300	EPJ	C11-N2-C10	3.00	120.23	116.37
2	C	300	EPJ	C11-N2-C10	3.04	120.28	116.37
2	D	300	EPJ	CL-C10-N2	3.07	122.47	116.10
2	C	300	EPJ	C8-C7-C11	3.17	120.05	116.83
2	B	300	EPJ	C11-N2-C10	4.47	122.13	116.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	EPJ	2	0
2	B	300	EPJ	6	0
2	C	300	EPJ	3	0
2	D	300	EPJ	2	0
2	E	300	EPJ	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	214/227 (94%)	-0.19	8 (3%) 42 38	30, 45, 90, 116	4 (1%)
1	B	214/227 (94%)	-0.23	5 (2%) 61 56	28, 43, 78, 101	2 (0%)
1	C	214/227 (94%)	-0.37	2 (0%) 84 80	27, 39, 72, 93	1 (0%)
1	D	214/227 (94%)	-0.35	8 (3%) 42 38	25, 38, 69, 94	1 (0%)
1	E	213/227 (93%)	-0.29	3 (1%) 75 71	25, 39, 79, 107	0
All	All	1069/1135 (94%)	-0.28	26 (2%) 59 55	25, 41, 81, 116	8 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-5	ASP	4.9
1	A	-5	ASP	3.7
1	D	-3	ASP	3.7
1	B	-5	ASP	3.6
1	A	-3	ASP	3.4
1	A	18	PRO	3.4
1	E	-3	ASP	3.1
1	A	-2	ASP	3.0
1	A	-1	LYS	2.8
1	C	68	ASP	2.8
1	B	70[A]	ASN	2.6
1	C	-5	ASP	2.6
1	A	-4	ASP	2.6
1	D	-4	ASP	2.5
1	E	70	ASN	2.5
1	E	-4	ASP	2.5
1	A	1	HIS	2.3
1	A	17	SER	2.2
1	B	74	ASN	2.2
1	D	1	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	-1	LYS	2.2
1	B	-3	ASP	2.2
1	B	-4	ASP	2.1
1	D	45	SER	2.1
1	D	-2	ASP	2.0
1	D	5	ASN	2.0

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EPJ	E	300	14/14	0.98	0.17	0.94	39,40,41,42	0
2	EPJ	A	300	14/14	0.97	0.17	0.19	44,45,45,46	0
2	EPJ	B	300	14/14	0.98	0.18	0.15	39,42,44,45	0
2	EPJ	D	300	14/14	0.98	0.14	-0.86	32,34,36,37	0
2	EPJ	C	300	14/14	0.97	0.14	-0.94	27,29,30,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.