



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:07 PM GMT

PDB ID : 1PP0  
Title : volvatoxin A2 in monoclinic crystal  
Authors : Lin, S.-C.; Lo, Y.-C.; Lin, J.-Y.; Liaw, Y.-C.  
Deposited on : 2003-06-16  
Resolution : 1.42 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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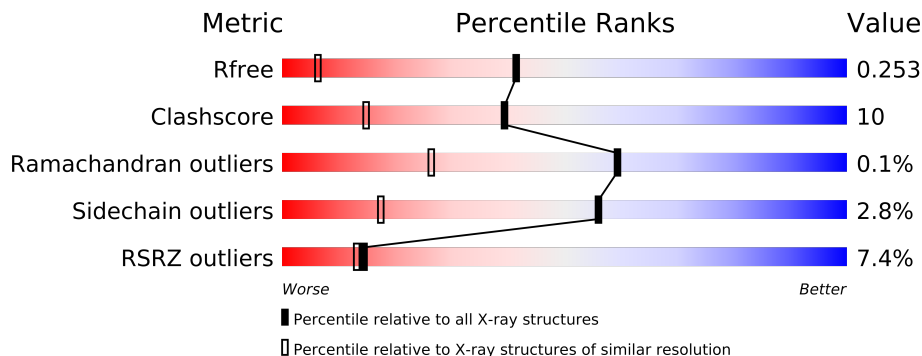
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.42 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))
$R_{free}$	66092	1110 (1.44-1.40)
Clashscore	79885	1263 (1.44-1.40)
Ramachandran outliers	78287	1226 (1.44-1.40)
Sidechain outliers	78261	1225 (1.44-1.40)
RSRZ outliers	66119	1110 (1.44-1.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	199	
1	B	199	
1	C	199	
1	D	199	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ACY	A	4004	-	X
2	ACY	A	4005	-	X
2	ACY	B	4008	-	X
2	ACY	D	4013	-	X

## 2 Entry composition i

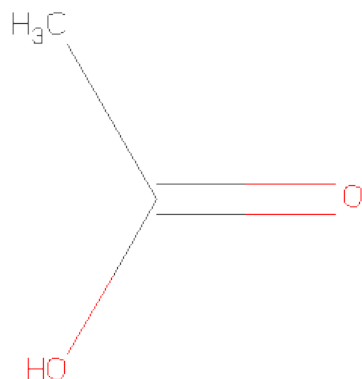
There are 3 unique types of molecules in this entry. The entry contains 6956 atoms, of which 0 are hydrogen and 0 are deuterium.

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 volvatoxin A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1527	994	237	295	1			
1	B	194	Total	C	N	O	S	0	0	0
			1547	1004	241	301	1			
1	C	194	Total	C	N	O	S	0	0	0
			1547	1004	241	301	1			
1	D	191	Total	C	N	O	S	0	0	0
			1527	994	237	295	1			

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

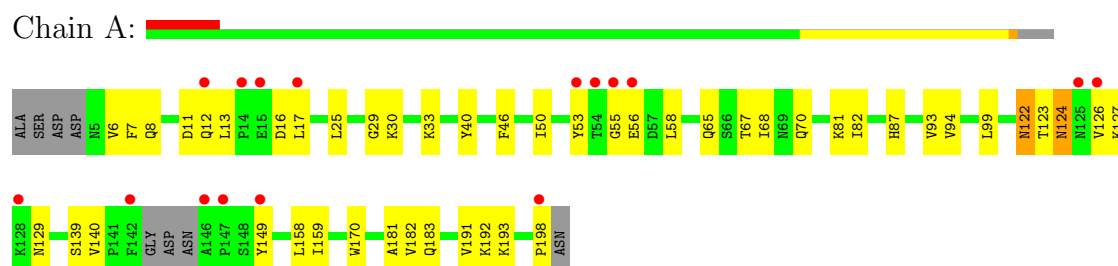
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	170	Total O 170 170	0	0
3	B	204	Total O 204 204	0	0
3	C	199	Total O 199 199	0	0
3	D	183	Total O 183 183	0	0

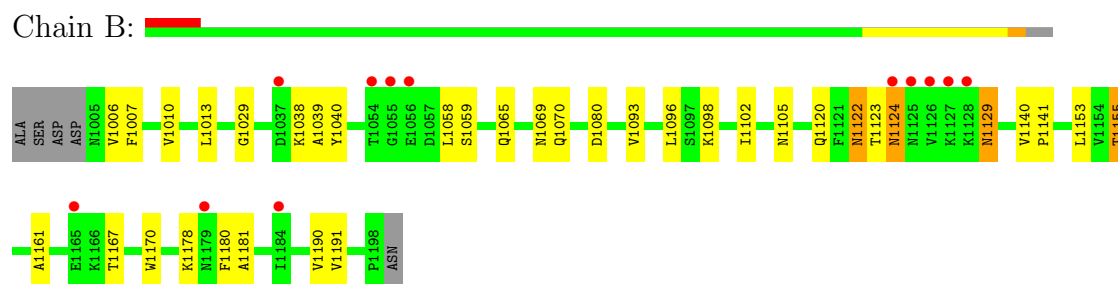
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

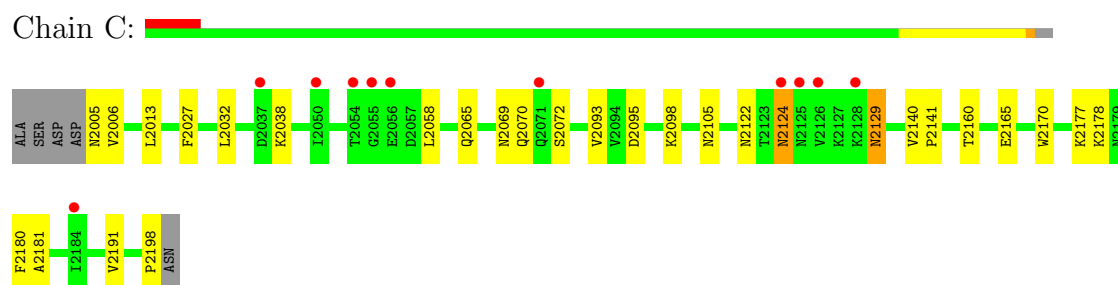
#### • Molecule 1: volvatoxin A2



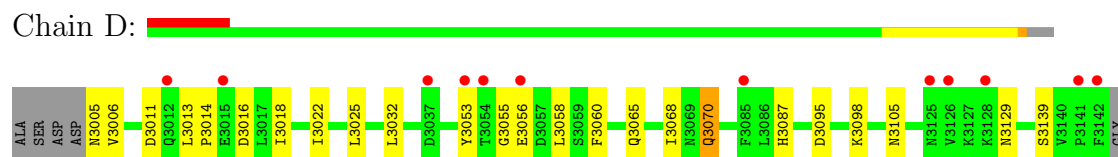
#### • Molecule 1: volvatoxin A2



#### • Molecule 1: volvatoxin A2



#### • Molecule 1: volvatoxin A2





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.98Å 57.48Å 114.63Å 90.00° 119.39° 90.00°	Depositor
Resolution (Å)	29.85 – 1.42 29.85 – 1.40	Depositor EDS
% Data completeness (in resolution range)	82.7 (29.85-1.42) 80.6 (29.85-1.40)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 1.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.229 , 0.255 0.228 , 0.253	Depositor DCC
$R_{free}$ test set	6898 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 146871 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.91 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2204e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.36	0/1563	0.59	0/2120
1	B	0.37	0/1584	0.60	0/2150
1	C	0.36	0/1584	0.60	0/2150
1	D	0.37	0/1563	0.60	0/2120
All	All	0.36	0/6294	0.60	0/8540

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1527	0	1501	41	0
1	B	1547	0	1515	35	0
1	C	1547	0	1515	22	0
1	D	1527	0	1501	23	0
2	A	20	0	15	3	0
2	B	12	0	9	2	0
2	C	4	0	3	0	0
2	D	16	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	170	0	0	7	1
3	B	204	0	0	4	1
3	C	199	0	0	3	0
3	D	183	0	0	4	0
All	All	6956	0	6071	118	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (118) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2105:ASN:HB3	3:C:5712:HOH:O	1.64	0.97
1:A:94:VAL:HG21	1:A:99:LEU:HD22	1.54	0.88
1:A:65:GLN:HE21	1:B:1065:GLN:NE2	1.72	0.87
1:C:2070:GLN:HG3	1:C:2181:ALA:HB2	1.55	0.86
1:A:12:GLN:HA	3:A:5552:HOH:O	1.78	0.84
1:B:1010:VAL:HG12	2:B:4008:ACY:H2	1.66	0.76
2:A:4012:ACY:C	3:A:5194:HOH:O	2.35	0.75
1:D:3070:GLN:H	1:D:3070:GLN:HE21	1.33	0.74
1:A:124:ASN:C	1:A:124:ASN:HD22	1.94	0.71
1:A:33:LYS:HE3	3:A:5619:HOH:O	1.92	0.70
1:B:1070:GLN:HG3	1:B:1181:ALA:HB2	1.73	0.69
1:A:6:VAL:HG23	1:A:7:PHE:HD2	1.58	0.68
1:D:3005:ASN:HA	3:D:5516:HOH:O	1.93	0.68
1:B:1098:LYS:HE2	3:B:5671:HOH:O	1.93	0.68
1:A:94:VAL:CG2	1:A:99:LEU:HB2	2.25	0.66
1:B:1093:VAL:HA	1:B:1140:VAL:HG21	1.82	0.61
1:B:1038:LYS:HE2	1:B:1122:ASN:ND2	2.15	0.61
1:D:3087:HIS:HD2	3:D:5036:HOH:O	1.84	0.60
3:A:5359:HOH:O	1:D:3087:HIS:HE1	1.84	0.60
1:B:1039:ALA:H	1:B:1120:GLN:NE2	1.99	0.60
1:D:3105:ASN:HB3	3:D:5637:HOH:O	2.01	0.60
1:B:1124:ASN:HB3	1:B:1129:ASN:ND2	2.17	0.59
1:B:1096:LEU:C	1:B:1096:LEU:HD13	2.23	0.58
1:A:159:ILE:HD13	1:A:182:VAL:HG13	1.83	0.58
1:D:3146:ALA:N	1:D:3147:PRO:HD2	2.19	0.58
1:A:70:GLN:HG3	1:A:181:ALA:HB2	1.85	0.58
1:B:1105:ASN:HB3	3:B:5740:HOH:O	2.03	0.58
1:A:53:TYR:CE2	1:A:58:LEU:HB3	2.38	0.58
1:C:2129:ASN:C	1:C:2129:ASN:HD22	2.08	0.57
1:C:2105:ASN:ND2	3:C:5459:HOH:O	2.38	0.56
1:D:3165:GLU:H	2:D:4001:ACY:H3	1.71	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2178:LYS:HB2	1:C:2180:PHE:CE2	2.40	0.56
1:A:67:THR:OG1	1:A:183:GLN:NE2	2.38	0.56
1:D:3070:GLN:H	1:D:3070:GLN:NE2	2.04	0.55
1:D:3053:TYR:CE2	1:D:3058:LEU:HB3	2.42	0.55
1:B:1006:VAL:HG21	1:B:1029:GLY:HA2	1.89	0.55
1:B:1006:VAL:HG23	1:B:1007:PHE:HD2	1.71	0.55
1:A:53:TYR:CZ	1:A:55:GLY:HA3	2.44	0.53
1:C:2093:VAL:HA	1:C:2140:VAL:HG21	1.90	0.53
1:A:8:GLN:NE2	2:A:4004:ACY:OXT	2.42	0.53
1:C:2070:GLN:CG	1:C:2181:ALA:HB2	2.35	0.53
1:D:3068:ILE:HD11	3:D:5276:HOH:O	2.09	0.52
1:A:122:ASN:HD22	1:A:123:THR:H	1.57	0.52
1:D:3018:ILE:O	1:D:3022:ILE:HG12	2.10	0.52
1:B:1070:GLN:HE21	1:B:1181:ALA:CB	2.23	0.52
1:D:3053:TYR:CZ	1:D:3055:GLY:HA3	2.45	0.52
1:B:1167:THR:HG23	3:B:5656:HOH:O	2.10	0.51
1:C:2124:ASN:HB3	1:C:2129:ASN:ND2	2.25	0.51
1:B:1129:ASN:C	1:B:1129:ASN:HD22	2.13	0.51
1:C:2006:VAL:HG13	1:C:2032:LEU:HD22	1.93	0.51
1:A:65:GLN:HG2	1:B:1065:GLN:HB3	1.93	0.50
1:C:2177:LYS:HD2	3:C:5648:HOH:O	2.11	0.50
1:B:1058:LEU:HD12	1:B:1191:VAL:HG22	1.93	0.50
1:A:94:VAL:HG21	1:A:99:LEU:HB2	1.93	0.50
1:B:1070:GLN:CD	1:B:1070:GLN:H	2.14	0.49
1:A:124:ASN:ND2	1:A:127:LYS:H	2.11	0.49
1:B:1038:LYS:HE2	1:B:1122:ASN:HD21	1.78	0.49
1:A:11:ASP:HB3	1:A:139:SER:HB2	1.95	0.48
1:B:1080:ASP:CG	3:B:5715:HOH:O	2.50	0.48
1:B:1122:ASN:ND2	1:B:1123:THR:H	2.11	0.48
1:A:6:VAL:HG21	1:A:29:GLY:HA2	1.94	0.48
1:A:68:ILE:HD12	1:A:68:ILE:N	2.29	0.48
1:B:1153:LEU:HG	1:B:1155:THR:HG22	1.96	0.48
1:B:1010:VAL:HG11	1:B:1102:ILE:HD13	1.95	0.47
1:D:3014:PRO:HB2	1:D:3016:ASP:OD1	2.14	0.47
1:A:122:ASN:ND2	1:A:123:THR:H	2.13	0.47
1:D:3011:ASP:HB3	1:D:3139:SER:HB2	1.96	0.47
1:C:2013:LEU:HD23	1:C:2141:PRO:HD3	1.96	0.47
1:A:124:ASN:HD21	1:A:126:VAL:HB	1.79	0.46
1:C:2027:PHE:CD1	1:C:2198:PRO:HD2	2.50	0.46
1:B:1010:VAL:CG1	2:B:4008:ACY:H2	2.41	0.46
1:C:2095:ASP:OD1	1:C:2098:LYS:HB2	2.15	0.46
1:B:1070:GLN:HE21	1:B:1181:ALA:HB2	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1122:ASN:HD22	1:B:1123:THR:H	1.64	0.46
1:A:58:LEU:HD12	1:A:191:VAL:HG22	1.98	0.45
1:C:2072:SER:OG	1:C:2177:LYS:HE3	2.17	0.45
1:D:3095:ASP:HB3	1:D:3098:LYS:HB3	1.98	0.45
1:A:124:ASN:C	1:A:124:ASN:ND2	2.67	0.45
1:A:87:HIS:HE1	3:A:5359:HOH:O	1.99	0.45
1:B:1039:ALA:H	1:B:1120:GLN:HE21	1.65	0.45
1:A:16:ASP:CG	1:A:17:LEU:HD22	2.37	0.45
1:D:3070:GLN:N	1:D:3070:GLN:HE21	2.10	0.45
1:C:2058:LEU:HD12	1:C:2191:VAL:HG22	1.98	0.45
1:D:3070:GLN:CD	1:D:3181:ALA:HB2	2.37	0.45
1:D:3013:LEU:HD11	1:D:3139:SER:HB3	1.99	0.45
1:A:94:VAL:HG21	1:A:99:LEU:CD2	2.37	0.44
1:A:6:VAL:HG23	1:A:7:PHE:CD2	2.46	0.44
1:D:3129:ASN:HB2	1:D:3161:ALA:O	2.18	0.44
1:D:3006:VAL:HG13	1:D:3032:LEU:HD22	1.98	0.44
1:B:1124:ASN:HB3	1:B:1129:ASN:HD21	1.82	0.44
1:B:1178:LYS:HB2	1:B:1180:PHE:CE2	2.53	0.44
1:C:2038:LYS:HE2	1:C:2122:ASN:OD1	2.17	0.44
1:A:17:LEU:CD1	1:A:193:LYS:HB2	2.48	0.44
1:B:1129:ASN:HB2	1:B:1161:ALA:O	2.17	0.43
1:A:149:TYR:CE1	1:A:192:LYS:HB2	2.53	0.43
1:C:2069:ASN:HB2	1:D:3060:PHE:CD2	2.53	0.43
1:A:81:LYS:HB3	3:A:5344:HOH:O	2.18	0.43
1:C:2129:ASN:C	1:C:2129:ASN:ND2	2.70	0.43
1:A:13:LEU:HD11	1:A:139:SER:HB3	2.01	0.43
1:C:2058:LEU:CD1	1:C:2191:VAL:HG22	2.49	0.43
1:B:1013:LEU:HD23	1:B:1141:PRO:HD3	2.00	0.43
1:C:2070:GLN:OE1	1:C:2070:GLN:N	2.48	0.42
1:B:1058:LEU:CD1	1:B:1191:VAL:HG22	2.49	0.42
1:C:2065:GLN:HB3	1:D:3065:GLN:HG2	2.02	0.42
1:A:30:LYS:NZ	1:A:198:PRO:O	2.53	0.42
1:B:1040:TYR:OH	1:B:1122:ASN:HB2	2.21	0.41
1:A:127:LYS:HG2	3:A:5733:HOH:O	2.19	0.41
1:A:93:VAL:HA	1:A:140:VAL:HG21	2.03	0.41
1:A:46:PHE:CZ	1:A:50:ILE:HD11	2.56	0.41
1:A:40:TYR:OH	1:A:122:ASN:HB2	2.20	0.41
1:B:1059:SER:OG	1:B:1190:VAL:HB	2.20	0.41
1:B:1129:ASN:C	1:B:1129:ASN:ND2	2.74	0.41
1:A:82:ILE:HD11	1:A:159:ILE:HD11	2.02	0.41
1:D:3146:ALA:N	1:D:3147:PRO:CD	2.83	0.41
1:A:124:ASN:HB3	1:A:129:ASN:OD1	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2160:THR:HB	1:C:2181:ALA:HB3	2.04	0.40
1:A:158:LEU:HD11	2:A:4005:ACY:H3	2.04	0.40
1:A:158:LEU:HB3	1:A:183:GLN:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:5232:HOH:O	3:B:5360:HOH:O[4.546]	2.11	0.09

## 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	187/199 (94%)	180 (96%)	6 (3%)	1 (0%)	38	11
1	B	192/199 (96%)	188 (98%)	4 (2%)	0	100	100
1	C	192/199 (96%)	189 (98%)	3 (2%)	0	100	100
1	D	187/199 (94%)	181 (97%)	6 (3%)	0	100	100
All	All	758/796 (95%)	738 (97%)	19 (2%)	1 (0%)	59	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	GLU

### 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	169/175 (97%)	165 (98%)	4 (2%)	61	23
1	B	171/175 (98%)	165 (96%)	6 (4%)	48	12
1	C	171/175 (98%)	166 (97%)	5 (3%)	55	17
1	D	169/175 (97%)	165 (98%)	4 (2%)	61	23
All	All	680/700 (97%)	661 (97%)	19 (3%)	56	17

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	122	ASN
1	A	124	ASN
1	A	170	TRP
1	B	1069	ASN
1	B	1122	ASN
1	B	1124	ASN
1	B	1129	ASN
1	B	1155	THR
1	B	1170	TRP
1	C	2005	ASN
1	C	2124	ASN
1	C	2129	ASN
1	C	2165	GLU
1	C	2170	TRP
1	D	3025	LEU
1	D	3056	GLU
1	D	3070	GLN
1	D	3170	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	52	ASN
1	A	71	GLN
1	A	87	HIS
1	A	122	ASN
1	A	124	ASN
1	A	183	GLN
1	B	1005	ASN

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Mol	Chain	Res	Type
1	B	1036	GLN
1	B	1065	GLN
1	B	1069	ASN
1	B	1070	GLN
1	B	1071	GLN
1	B	1105	ASN
1	B	1120	GLN
1	B	1122	ASN
1	B	1124	ASN
1	B	1129	ASN
1	B	1145	ASN
1	C	2005	ASN
1	C	2105	ASN
1	C	2109	ASN
1	C	2124	ASN
1	C	2129	ASN
1	C	2183	GLN
1	D	3036	GLN
1	D	3052	ASN
1	D	3065	GLN
1	D	3070	GLN
1	D	3071	GLN
1	D	3073	GLN
1	D	3087	HIS
1	D	3125	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

13 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	ACY	A	4003	-	3,3,3	1.01	0	3,3,3	1.45	0
2	ACY	A	4004	-	3,3,3	1.04	0	3,3,3	1.49	1 (33%)
2	ACY	A	4005	-	3,3,3	1.04	0	3,3,3	1.46	0
2	ACY	A	4011	-	3,3,3	1.03	0	3,3,3	1.45	0
2	ACY	A	4012	-	3,3,3	1.04	0	3,3,3	1.46	0
2	ACY	B	4002	-	3,3,3	1.04	0	3,3,3	1.42	0
2	ACY	B	4007	-	3,3,3	0.95	0	3,3,3	1.43	0
2	ACY	B	4008	-	3,3,3	1.00	0	3,3,3	1.45	0
2	ACY	C	4006	-	3,3,3	1.01	0	3,3,3	1.43	0
2	ACY	D	4001	-	3,3,3	1.18	0	3,3,3	1.41	0
2	ACY	D	4009	-	3,3,3	1.04	0	3,3,3	1.41	0
2	ACY	D	4010	-	3,3,3	1.00	0	3,3,3	1.46	0
2	ACY	D	4013	-	3,3,3	1.04	0	3,3,3	1.47	1 (33%)

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	ACY	A	4003	-	-	0/0/0/0	0/0/0/0
2	ACY	A	4004	-	-	0/0/0/0	0/0/0/0
2	ACY	A	4005	-	-	0/0/0/0	0/0/0/0
2	ACY	A	4011	-	-	0/0/0/0	0/0/0/0
2	ACY	A	4012	-	-	0/0/0/0	0/0/0/0
2	ACY	B	4002	-	-	0/0/0/0	0/0/0/0
2	ACY	B	4007	-	-	0/0/0/0	0/0/0/0
2	ACY	B	4008	-	-	0/0/0/0	0/0/0/0
2	ACY	C	4006	-	-	0/0/0/0	0/0/0/0
2	ACY	D	4001	-	-	0/0/0/0	0/0/0/0
2	ACY	D	4009	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACY	D	4010	-	-	0/0/0/0	0/0/0/0
2	ACY	D	4013	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4004	ACY	O-C-CH3	-2.02	113.24	122.06
2	D	4013	ACY	O-C-CH3	-2.00	113.32	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	191/199 (95%)	0.67	16 (8%) 11 10	16, 26, 53, 82	0
1	B	194/199 (97%)	0.55	12 (6%) 20 19	15, 25, 46, 65	0
1	C	194/199 (97%)	0.50	11 (5%) 23 22	15, 24, 47, 67	0
1	D	191/199 (95%)	0.65	17 (8%) 10 9	16, 25, 53, 72	0
All	All	770/796 (96%)	0.59	56 (7%) 14 13	15, 25, 51, 82	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	ALA	9.7
1	C	2126	VAL	8.8
1	B	1126	VAL	8.6
1	D	3146	ALA	7.1
1	D	3142	PHE	6.8
1	A	56	GLU	6.2
1	C	2125	ASN	6.0
1	A	54	THR	5.4
1	A	126	VAL	5.3
1	D	3054	THR	5.1
1	B	1125	ASN	5.0
1	D	3126	VAL	5.0
1	A	147	PRO	4.7
1	D	3147	PRO	4.7
1	D	3056	GLU	4.4
1	D	3125	ASN	4.2
1	D	3012	GLN	4.2
1	B	1128	LYS	4.0
1	B	1056	GLU	4.0
1	B	1054	THR	3.9
1	A	12	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	142	PHE	3.7
1	B	1055	GLY	3.6
1	C	2055	GLY	3.6
1	A	125	ASN	3.4
1	D	3128	LYS	3.3
1	D	3141	PRO	3.3
1	C	2128	LYS	3.0
1	B	1037	ASP	3.0
1	A	55	GLY	2.9
1	D	3198	PRO	2.8
1	C	2056	GLU	2.8
1	B	1127	LYS	2.6
1	A	198	PRO	2.6
1	D	3015	GLU	2.5
1	A	53	TYR	2.5
1	A	149	TYR	2.5
1	C	2184	ILE	2.4
1	B	1124	ASN	2.4
1	C	2054	THR	2.4
1	A	14	PRO	2.3
1	A	128	LYS	2.3
1	C	2037	ASP	2.3
1	D	3037	ASP	2.2
1	D	3053	TYR	2.2
1	D	3149	TYR	2.2
1	A	17	LEU	2.2
1	B	1165	GLU	2.2
1	C	2124	ASN	2.1
1	B	1184	ILE	2.1
1	B	1179	ASN	2.1
1	A	15	GLU	2.1
1	D	3184	ILE	2.0
1	D	3085	PHE	2.0
1	C	2050	ILE	2.0
1	C	2071	GLN	2.0

## 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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACY	A	4005	4/4	0.42	19.38	81,82,82,83	0
2	ACY	A	4004	4/4	0.21	8.01	68,68,70,71	0
2	ACY	D	4013	4/4	0.34	4.71	116,116,116,116	0
2	ACY	B	4008	4/4	0.23	2.92	74,74,75,75	0
2	ACY	D	4001	4/4	0.17	1.98	34,37,41,42	0
2	ACY	A	4012	4/4	0.20	1.77	46,46,48,49	0
2	ACY	D	4009	4/4	0.15	1.51	38,40,41,44	0
2	ACY	D	4010	4/4	0.26	1.19	53,53,53,54	0
2	ACY	B	4007	4/4	0.15	1.02	43,44,46,47	0
2	ACY	A	4011	4/4	0.20	0.83	55,56,57,57	0
2	ACY	A	4003	4/4	0.13	0.45	40,41,44,48	0
2	ACY	C	4006	4/4	0.11	-0.03	32,33,34,41	0
2	ACY	B	4002	4/4	0.10	-1.00	31,32,34,37	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.