



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:52 PM UTC

PDB ID : 1PP0 / pdb_00001pp0
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 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

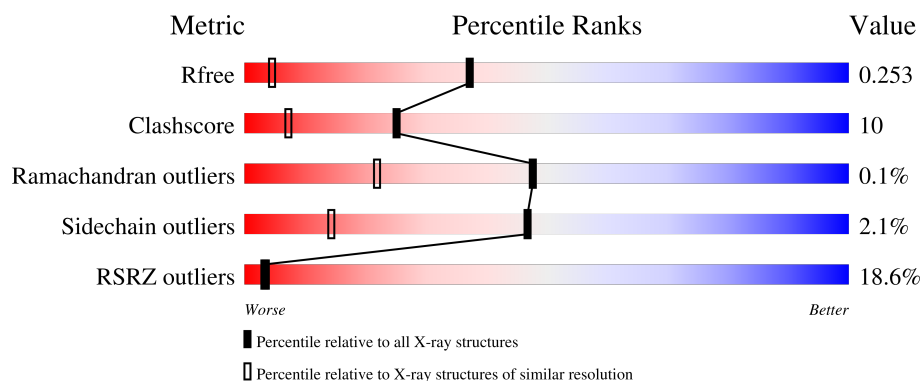
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (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 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 $\leq 5\%$. 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	199	20% 71% 23% ..
1	B	199	14% 78% 18% ..
1	C	199	16% 83% 14% ..
1	D	199	22% 81% 14% ..

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	ACY	B	4008	-	-	X	-

2 Entry composition [i](#)

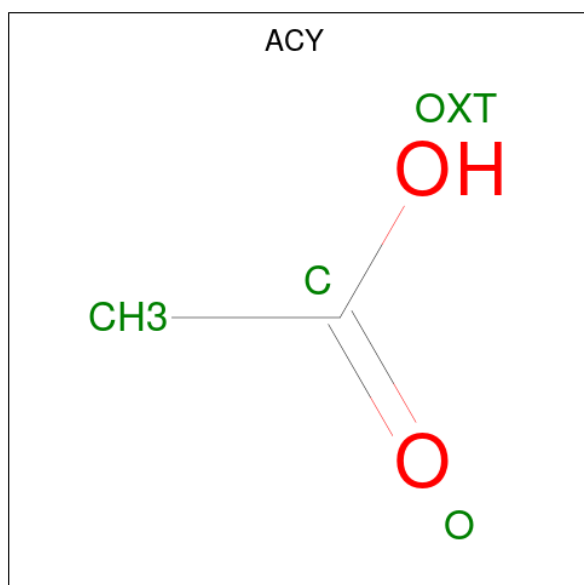
There are 3 unique types of molecules in this entry. The entry contains 6956 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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 (CCD ID: ACY) (formula: C₂H₄O₂).



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

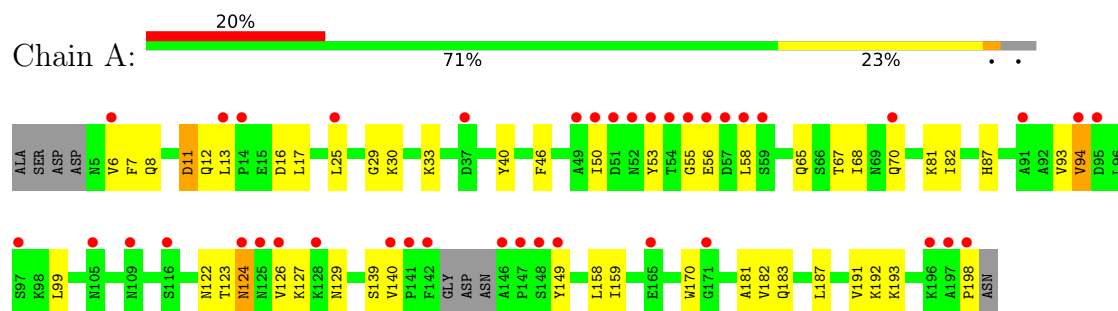
- Molecule 3 is water.

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

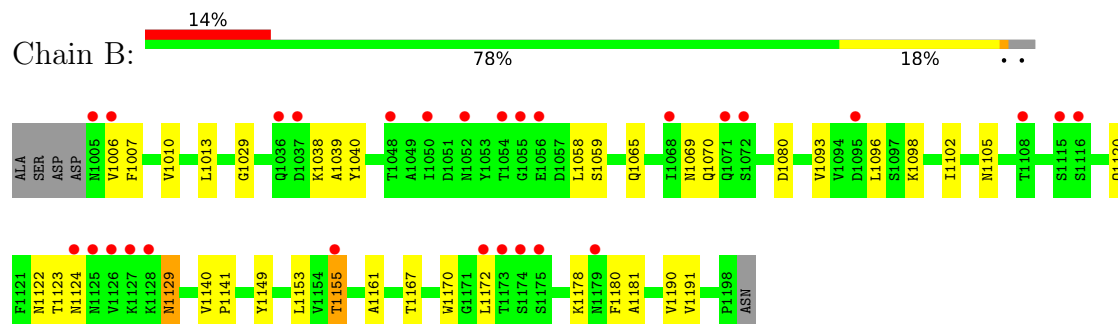
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

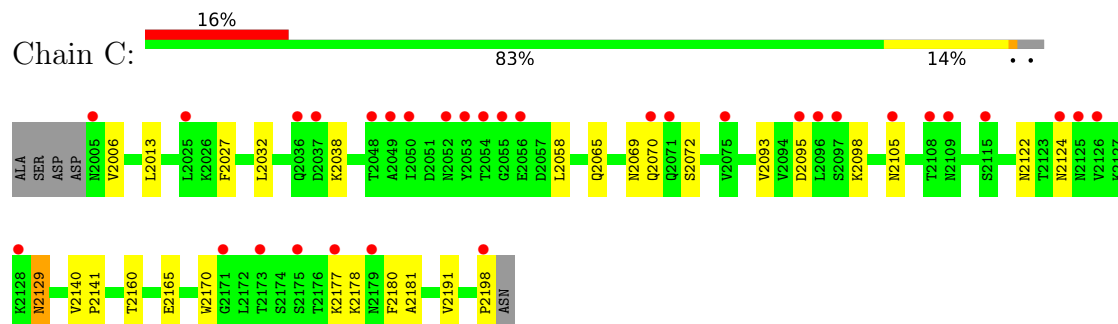
• Molecule 1: volvatoxin A2



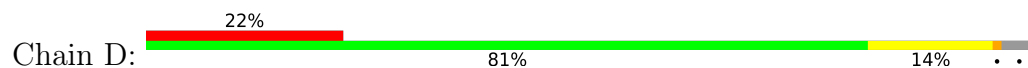
• Molecule 1: volvatoxin A2

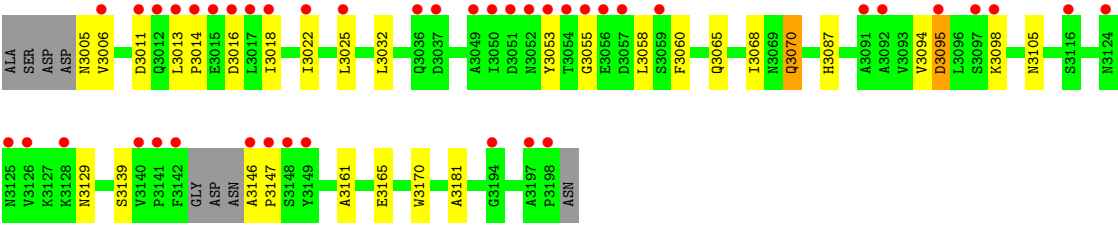


• Molecule 1: volvatoxin A2



• Molecule 1: volvatoxin A2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.98Å 57.48Å 114.63Å 90.00° 119.39° 90.00°	Depositor
Resolution (Å)	29.85 – 1.42 29.85 – 1.42	Depositor EDS
% Data completeness (in resolution range)	82.7 (29.85-1.42) 82.7 (29.85-1.42)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 1.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.255 0.227 , 0.253	Depositor DCC
R_{free} test set	6898 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6956	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.37	0/1563	0.81	2/2120 (0.1%)
1	B	0.39	0/1584	0.83	1/2150 (0.0%)
1	C	0.38	0/1584	0.82	0/2150
1	D	0.38	0/1563	0.81	2/2120 (0.1%)
All	All	0.38	0/6294	0.82	5/8540 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3094	VAL	N-CA-C	8.07	119.89	108.36
1	A	94	VAL	N-CA-C	7.28	118.96	108.48
1	A	11	ASP	N-CA-C	6.09	118.32	109.07
1	D	3095	ASP	N-CA-C	-5.37	99.98	108.73
1	B	1149	TYR	N-CA-C	5.12	117.92	109.72

There are no chirality outliers.

There are no planarity outliers.

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	1527	0	1501	41	0
1	B	1547	0	1515	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	119	1

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 (119) 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: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:A:124:ASN:C	1:A:124:ASN:HD22	1.94	0.76
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: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:B:1098:LYS:HE2	3:B:5671:HOH:O	1.93	0.68
1:D:3005:ASN:HA	3:D:5516:HOH:O	1.93	0.68
1:A:94:VAL:CG2	1:A:99:LEU:HB2	2.25	0.66
1:B:1096:LEU:C	1:B:1096:LEU:HD13	2.23	0.63
1:C:2129:ASN:HD22	1:C:2129:ASN:C	2.08	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1124:ASN:HB3	1:B:1129:ASN:ND2	2.17	0.59
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: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
1:A:67:THR:OG1	1:A:183:GLN:NE2	2.38	0.56
1:C:2178:LYS:HB2	1:C:2180:PHE:CE2	2.40	0.56
1:D:3053:TYR:CE2	1:D:3058:LEU:HB3	2.42	0.55
1:D:3070:GLN:H	1:D:3070:GLN:NE2	2.04	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:B:1080:ASP:CG	3:B:5715:HOH:O	2.50	0.54
1:B:1070:GLN:H	1:B:1070:GLN:CD	2.14	0.54
1:B:1129:ASN:C	1:B:1129:ASN:HD22	2.13	0.54
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: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:B:1058:LEU:HD12	1:B:1191:VAL:HG22	1.93	0.50
1:C:2177:LYS:HD2	3:C:5648:HOH:O	2.11	0.50
1:A:94:VAL:HG21	1:A:99:LEU:HB2	1.93	0.50
1:A:16:ASP:CG	1:A:17:LEU:HD22	2.37	0.50
1:D:3070:GLN:CD	1:D:3181:ALA:HB2	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:2013:LEU:HD23	1:C:2141:PRO:HD3	1.96	0.47
1:D:3011:ASP:HB3	1:D:3139:SER:HB2	1.96	0.47
1:C:2129:ASN:C	1:C:2129:ASN:ND2	2.70	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:1129:ASN:ND2	1:B:1129:ASN:C	2.74	0.46
1:B:1070:GLN:HE21	1:B:1181:ALA:HB2	1.80	0.46
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: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:C:2058:LEU:HD12	1:C:2191:VAL:HG22	1.98	0.45
1:D:3070:GLN:HE21	1:D:3070:GLN:N	2.10	0.45
1:D:3013:LEU:HD11	1:D:3139:SER:HB3	1.99	0.45
1:A:6:VAL:HG23	1:A:7:PHE:CD2	2.46	0.44
1:A:94:VAL:HG21	1:A:99:LEU:CD2	2.37	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:A:149:TYR:CE1	1:A:192:LYS:HB2	2.53	0.43
1:B:1129:ASN:HB2	1:B:1161:ALA:O	2.17	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:A:13:LEU:HD11	1:A:139:SER:HB3	2.01	0.43
1:B:1013:LEU:HD23	1:B:1141:PRO:HD3	2.00	0.43
1:C:2058:LEU:CD1	1:C:2191:VAL:HG22	2.49	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:B:1096:LEU:C	1:B:1096:LEU:CD1	2.91	0.42
1:C:2065:GLN:HB3	1:D:3065:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:46:PHE:CZ	1:A:50:ILE:HD11	2.56	0.41
1:A:93:VAL:HA	1:A:140:VAL:HG21	2.03	0.41
1:A:127:LYS:HG2	3:A:5733:HOH:O	2.19	0.41
1:A:40:TYR:OH	1:A:122:ASN:HB2	2.20	0.41
1:A:187:LEU:HD23	1:A:187:LEU:C	2.45	0.41
1:B:1059:SER:OG	1:B:1190:VAL:HB	2.20	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
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	Interatomic distance (Å)	Clash overlap (Å)
3:A:5232:HOH:O	3:B:5360:HOH:O[4_546]	2.11	0.09

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	187/199 (94%)	180 (96%)	6 (3%)	1 (0%)	24	7
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%)	48	22

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%)	166 (98%)	3 (2%)	51	18
1	B	171/175 (98%)	166 (97%)	5 (3%)	37	8
1	C	171/175 (98%)	168 (98%)	3 (2%)	51	18
1	D	169/175 (97%)	166 (98%)	3 (2%)	51	18
All	All	680/700 (97%)	666 (98%)	14 (2%)	47	14

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	124	ASN
1	A	170	TRP
1	B	1069	ASN
1	B	1129	ASN
1	B	1155	THR
1	B	1170	TRP
1	B	1172	LEU
1	C	2129	ASN
1	C	2165	GLU
1	C	2170	TRP
1	D	3025	LEU
1	D	3070	GLN
1	D	3170	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
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
1	B	1036	GLN
1	B	1065	GLN
1	B	1069	ASN
1	B	1070	GLN
1	B	1071	GLN
1	B	1073	GLN
1	B	1105	ASN
1	B	1109	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	2073	GLN
1	C	2105	ASN
1	C	2109	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	3073	GLN
1	D	3087	HIS
1	D	3125	ASN

5.3.3 RNA ⓘ

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](#)

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	4012	-	3,3,3	1.29	0	3,3,3	1.64	1 (33%)
2	ACY	C	4006	-	3,3,3	1.26	0	3,3,3	1.60	1 (33%)
2	ACY	B	4007	-	3,3,3	1.19	0	3,3,3	1.61	1 (33%)
2	ACY	A	4005	-	3,3,3	1.29	0	3,3,3	1.63	1 (33%)
2	ACY	B	4002	-	3,3,3	1.29	0	3,3,3	1.60	1 (33%)
2	ACY	A	4004	-	3,3,3	1.30	1 (33%)	3,3,3	1.67	1 (33%)
2	ACY	A	4011	-	3,3,3	1.29	1 (33%)	3,3,3	1.63	1 (33%)
2	ACY	D	4009	-	3,3,3	1.30	0	3,3,3	1.59	1 (33%)
2	ACY	D	4013	-	3,3,3	1.30	1 (33%)	3,3,3	1.65	1 (33%)
2	ACY	D	4001	-	3,3,3	1.45	1 (33%)	3,3,3	1.58	1 (33%)
2	ACY	B	4008	-	3,3,3	1.26	0	3,3,3	1.62	1 (33%)
2	ACY	A	4003	-	3,3,3	1.26	0	3,3,3	1.62	1 (33%)
2	ACY	D	4010	-	3,3,3	1.25	0	3,3,3	1.63	1 (33%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4001	ACY	O-C	2.19	1.31	1.22
2	A	4004	ACY	O-C	2.05	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4013	ACY	O-C	2.02	1.31	1.22
2	A	4011	ACY	O-C	2.02	1.31	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4004	ACY	O-C-CH3	-2.27	113.24	122.53
2	D	4013	ACY	O-C-CH3	-2.24	113.32	122.53
2	A	4012	ACY	O-C-CH3	-2.23	113.38	122.53
2	A	4005	ACY	O-C-CH3	-2.23	113.40	122.53
2	D	4010	ACY	O-C-CH3	-2.22	113.41	122.53
2	B	4008	ACY	O-C-CH3	-2.22	113.43	122.53
2	A	4011	ACY	O-C-CH3	-2.22	113.44	122.53
2	A	4003	ACY	O-C-CH3	-2.21	113.47	122.53
2	B	4007	ACY	O-C-CH3	-2.19	113.53	122.53
2	B	4002	ACY	O-C-CH3	-2.18	113.58	122.53
2	C	4006	ACY	O-C-CH3	-2.18	113.61	122.53
2	D	4009	ACY	O-C-CH3	-2.16	113.66	122.53
2	D	4001	ACY	O-C-CH3	-2.15	113.70	122.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4012	ACY	1	0
2	A	4005	ACY	1	0
2	A	4004	ACY	1	0
2	D	4001	ACY	1	0
2	B	4008	ACY	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/199 (95%)	1.20	40 (20%) 2 2	16, 26, 53, 82	0
1	B	194/199 (97%)	1.09	28 (14%) 6 7	15, 25, 46, 65	0
1	C	194/199 (97%)	0.98	32 (16%) 4 5	15, 24, 47, 67	0
1	D	191/199 (95%)	1.17	43 (22%) 2 2	16, 25, 53, 72	0
All	All	770/796 (96%)	1.11	143 (18%) 3 3	15, 25, 51, 82	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1126	VAL	6.3
1	D	3142	PHE	6.2
1	B	1055	GLY	5.9
1	A	146	ALA	5.8
1	B	1054	THR	5.5
1	A	147	PRO	5.5
1	C	2055	GLY	5.3
1	D	3147	PRO	5.3
1	D	3055	GLY	5.2
1	A	55	GLY	5.0
1	D	3126	VAL	4.9
1	C	2126	VAL	4.6
1	D	3146	ALA	4.6
1	A	54	THR	4.4
1	D	3014	PRO	4.3
1	B	1175	SER	4.2
1	A	53	TYR	4.0
1	D	3116	SER	3.9
1	D	3054	THR	3.9
1	B	1095	ASP	3.8
1	C	2125	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	3149	TYR	3.8
1	A	57	ASP	3.7
1	C	2198	PRO	3.7
1	A	126	VAL	3.6
1	A	142	PHE	3.5
1	A	197	ALA	3.5
1	B	1037	ASP	3.5
1	D	3052	ASN	3.5
1	D	3051	ASP	3.4
1	A	14	PRO	3.4
1	D	3059	SER	3.3
1	D	3125	ASN	3.3
1	B	1056	GLU	3.3
1	B	1116	SER	3.2
1	B	1124	ASN	3.2
1	B	1174	SER	3.2
1	C	2037	ASP	3.2
1	A	128	LYS	3.2
1	B	1036	GLN	3.2
1	D	3141	PRO	3.2
1	B	1125	ASN	3.2
1	B	1172	LEU	3.1
1	C	2054	THR	3.1
1	D	3037	ASP	3.1
1	A	94	VAL	3.1
1	B	1179	ASN	3.1
1	C	2050	ILE	3.1
1	D	3011	ASP	3.1
1	C	2071	GLN	3.0
1	A	198	PRO	3.0
1	D	3053	TYR	3.0
1	A	95	ASP	3.0
1	A	97	SER	2.9
1	A	52	ASN	2.9
1	C	2049	ALA	2.9
1	D	3092	ALA	2.9
1	B	1072	SER	2.9
1	C	2175	SER	2.9
1	A	141	PRO	2.8
1	A	125	ASN	2.8
1	A	58	LEU	2.8
1	D	3091	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	2036	GLN	2.8
1	C	2171	GLY	2.8
1	A	56	GLU	2.8
1	C	2124	ASN	2.8
1	A	49	ALA	2.7
1	C	2005	ASN	2.7
1	D	3140	VAL	2.7
1	C	2095	ASP	2.7
1	D	3022	ILE	2.7
1	A	149	TYR	2.7
1	B	1127	LYS	2.7
1	C	2052	ASN	2.7
1	C	2096	LEU	2.6
1	D	3057	ASP	2.6
1	B	1115	SER	2.6
1	B	1128	LYS	2.6
1	D	3056	GLU	2.5
1	A	59	SER	2.5
1	B	1173	THR	2.5
1	C	2048	THR	2.5
1	D	3049	ALA	2.5
1	A	6	VAL	2.5
1	C	2177	LYS	2.5
1	D	3006	VAL	2.5
1	A	70	GLN	2.5
1	C	2173	THR	2.5
1	D	3015	GLU	2.4
1	C	2097	SER	2.4
1	D	3194	GLY	2.4
1	A	196	LYS	2.4
1	D	3098	LYS	2.4
1	D	3095	ASP	2.4
1	B	1071	GLN	2.4
1	C	2070	GLN	2.4
1	A	37	ASP	2.4
1	D	3097	SER	2.4
1	A	105	ASN	2.4
1	B	1005	ASN	2.4
1	A	148	SER	2.3
1	D	3017	LEU	2.3
1	D	3050	ILE	2.3
1	C	2105	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	2179	ASN	2.3
1	C	2108	THR	2.3
1	C	2025	LEU	2.3
1	D	3197	ALA	2.2
1	B	1006	VAL	2.2
1	C	2056	GLU	2.2
1	A	116	SER	2.2
1	D	3013	LEU	2.2
1	D	3018	ILE	2.2
1	A	109	ASN	2.2
1	B	1052	ASN	2.2
1	C	2109	ASN	2.2
1	D	3016	ASP	2.2
1	A	51	ASP	2.2
1	D	3128	LYS	2.2
1	A	140	VAL	2.2
1	A	91	ALA	2.1
1	A	50	ILE	2.1
1	B	1068	ILE	2.1
1	B	1048	THR	2.1
1	D	3148	SER	2.1
1	D	3036	GLN	2.1
1	C	2128	LYS	2.1
1	D	3012	GLN	2.1
1	B	1108	THR	2.1
1	A	171	GLY	2.1
1	A	124	ASN	2.1
1	C	2053	TYR	2.1
1	A	165	GLU	2.1
1	C	2115	SER	2.1
1	D	3198	PRO	2.1
1	B	1155	THR	2.0
1	A	13	LEU	2.0
1	D	3025	LEU	2.0
1	B	1050	ILE	2.0
1	C	2075	VAL	2.0
1	A	25	LEU	2.0
1	D	3124	ASN	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 [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	ACY	D	4013	4/4	0.66	0.22	116,116,116,116	0
2	ACY	D	4001	4/4	0.68	0.16	34,37,41,42	0
2	ACY	A	4005	4/4	0.73	0.15	81,82,82,83	0
2	ACY	A	4012	4/4	0.73	0.16	46,46,48,49	0
2	ACY	B	4007	4/4	0.75	0.18	43,44,46,47	0
2	ACY	A	4004	4/4	0.76	0.15	68,68,70,71	0
2	ACY	B	4008	4/4	0.80	0.20	74,74,75,75	0
2	ACY	D	4010	4/4	0.81	0.12	53,53,53,54	0
2	ACY	A	4011	4/4	0.83	0.11	55,56,57,57	0
2	ACY	C	4006	4/4	0.88	0.10	32,33,34,41	0
2	ACY	D	4009	4/4	0.89	0.11	38,40,41,44	0
2	ACY	A	4003	4/4	0.90	0.10	40,41,44,48	0
2	ACY	B	4002	4/4	0.91	0.09	31,32,34,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.