



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 09:47 PM BST

PDB ID : 5T0W
Title : Crystal structure of the ancestral amino acid-binding protein AncCDT-1, a precursor of cyclohexadienyl dehydratase
Authors : Clifton, B.E.; Carr, P.D.; Jackson, C.J.
Deposited on : 2016-08-16
Resolution : 2.59 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
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) : 2.14.4.dev1

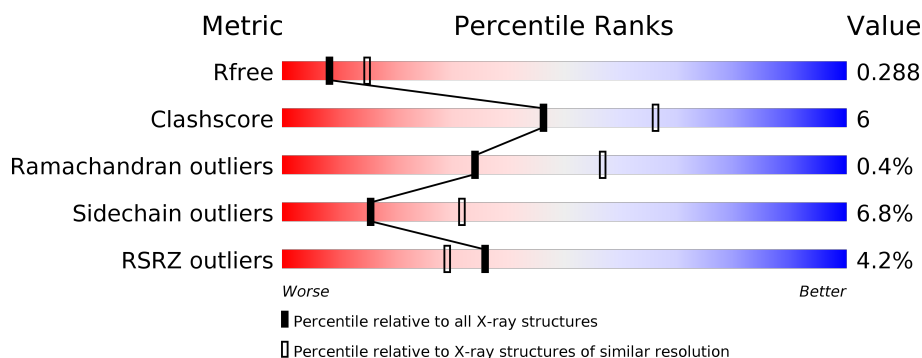
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 ≥ 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	247	<div> <div>5%</div> <div>74% 15% • 7%</div> </div>
1	B	247	<div> <div>5%</div> <div>77% 13% • 8%</div> </div>
1	C	247	<div> <div>6%</div> <div>77% 14% • 7%</div> </div>
1	D	247	<div> <div>4%</div> <div>74% 16% • 9%</div> </div>

2 Entry composition [i](#)

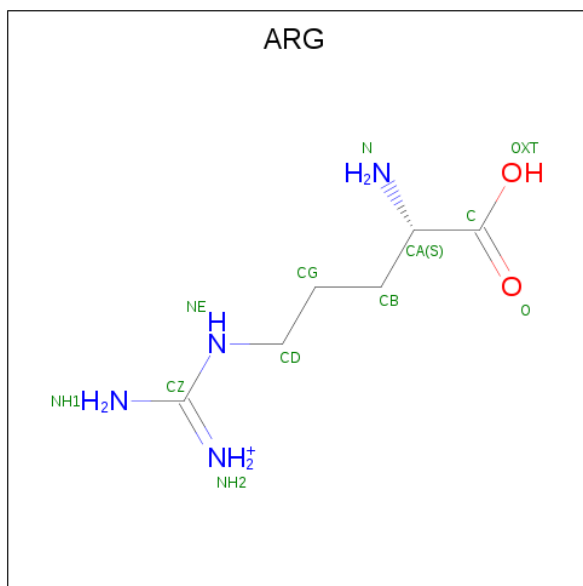
There are 3 unique types of molecules in this entry. The entry contains 7011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AncCDT-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1769	1136	287	340	6			
1	B	227	Total	C	N	O	S	0	0	0
			1734	1118	281	329	6			
1	C	229	Total	C	N	O	S	0	0	0
			1718	1106	276	330	6			
1	D	225	Total	C	N	O	S	0	1	0
			1721	1103	282	330	6			

- Molecule 2 is ARGinine (three-letter code: ARG) (formula: C₆H₁₅N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	4	2		
2	B	1	Total	C	N	O	0	0
			12	6	4	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			12	6	4	2		
2	D	1	Total	C	N	O	0	0
			12	6	4	2		

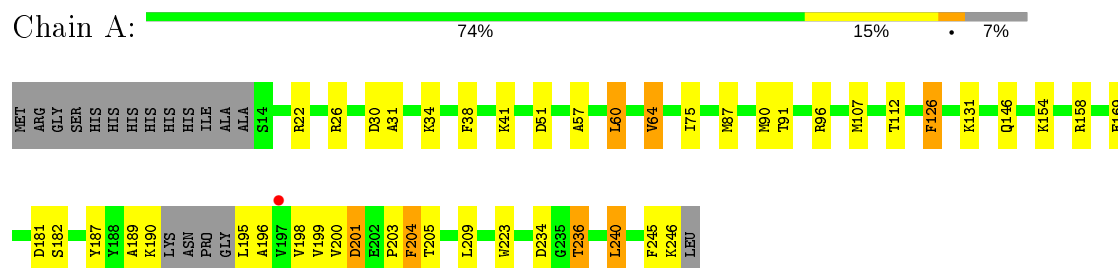
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	3	Total	O	0	0
			3	3		
3	D	7	Total	O	0	0
			7	7		

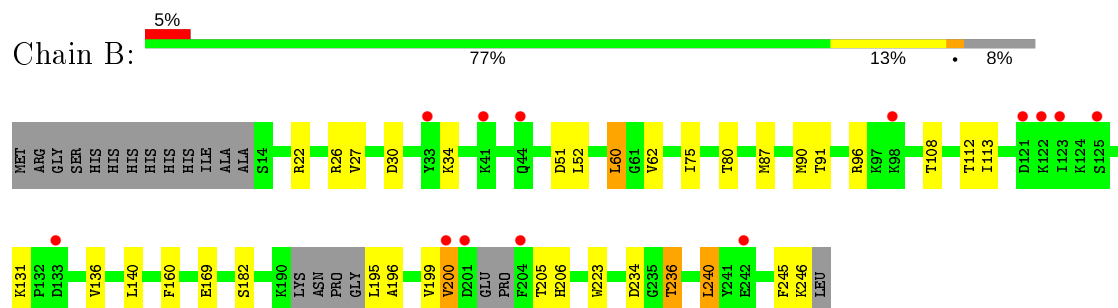
3 Residue-property plots [i](#)

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.

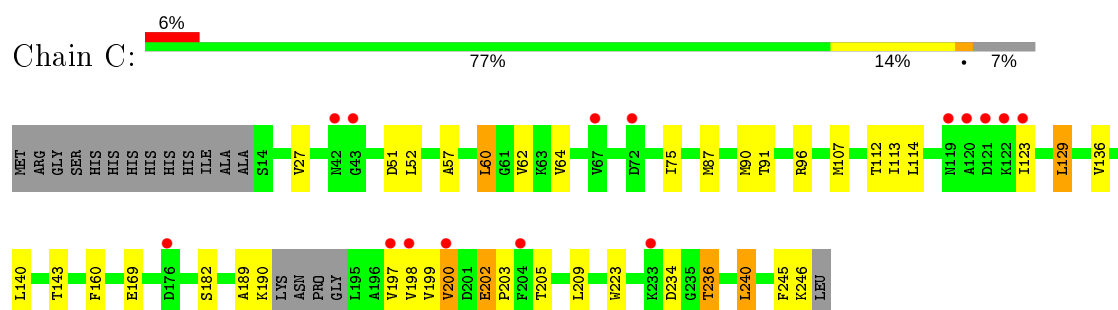
• Molecule 1: AncCDT-1



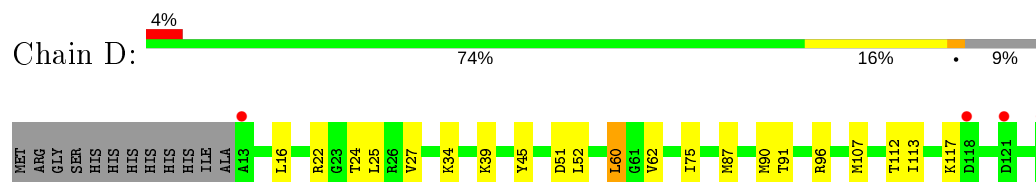
• Molecule 1: AncCDT-1

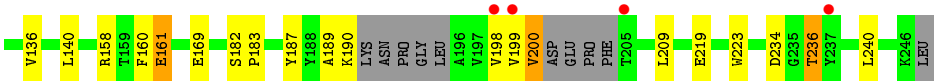


• Molecule 1: AncCDT-1



• Molecule 1: AncCDT-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.03Å 68.88Å 318.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.19 – 2.59 33.17 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.9 (33.19-2.59) 99.1 (33.17-2.59)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.253 , 0.287 0.254 , 0.288	Depositor DCC
R_{free} test set	1686 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7011	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.65	0/1807	0.76	5/2453 (0.2%)
1	B	0.52	0/1770	0.67	0/2402
1	C	0.47	0/1756	0.64	0/2395
1	D	0.57	0/1758	0.69	0/2386
All	All	0.56	0/7091	0.69	5/9636 (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	A	126	PHE	CB-CG-CD2	-6.62	116.16	120.80
1	A	200	VAL	CB-CA-C	-5.51	100.94	111.40
1	A	126	PHE	CB-CG-CD1	5.43	124.60	120.80
1	A	87	MET	CG-SD-CE	5.09	108.35	100.20
1	A	64	VAL	CB-CA-C	-5.07	101.76	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1769	0	1717	25	0
1	B	1734	0	1680	19	0
1	C	1718	0	1618	22	0
1	D	1721	0	1668	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	12	0	12	2	0
2	B	12	0	12	2	0
2	C	12	0	12	2	0
2	D	12	0	12	1	0
3	A	11	0	0	1	0
3	B	3	0	0	0	0
3	D	7	0	0	0	0
All	All	7011	0	6731	87	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.

All (87) 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:A:31:ALA:O	1:A:38:PHE:HA	1.88	0.74
1:B:160:PHE:CZ	1:B:169:GLU:HG3	2.23	0.73
1:A:203:PRO:O	1:A:204:PHE:CD2	2.43	0.72
1:D:160:PHE:CZ	1:D:169:GLU:HG3	2.26	0.71
1:B:234:ASP:OD1	1:B:236:THR:OG1	2.10	0.70
1:D:234:ASP:OD1	1:D:236:THR:OG1	2.10	0.69
1:C:160:PHE:CZ	1:C:169:GLU:HG3	2.27	0.69
1:C:234:ASP:OD1	1:C:236:THR:OG1	2.09	0.68
1:A:234:ASP:OD1	1:A:236:THR:OG1	2.11	0.68
1:C:91:THR:HG1	2:C:301:ARG:N	1.95	0.65
1:A:38:PHE:HB2	3:A:406:HOH:O	1.96	0.65
1:A:203:PRO:O	1:A:204:PHE:CG	2.50	0.64
1:C:114:LEU:HG	1:C:197:VAL:CG1	2.28	0.63
1:C:202:GLU:CB	1:C:203:PRO:CD	2.79	0.60
1:C:51:ASP:CB	1:C:240:LEU:HD21	2.31	0.59
1:B:51:ASP:CB	1:B:240:LEU:HD21	2.33	0.59
1:B:245:PHE:O	1:B:246:LYS:C	2.41	0.59
1:A:34:LYS:HD2	1:A:187:TYR:CE1	2.39	0.58
1:B:108:THR:HG22	1:B:206:HIS:ND1	2.19	0.57
1:A:245:PHE:O	1:A:246:LYS:C	2.43	0.57
1:D:60:LEU:HD13	1:D:223:TRP:NE1	2.20	0.56
1:B:34:LYS:HZ1	1:D:219:GLU:CD	2.09	0.56
1:A:60:LEU:HD13	1:A:223:TRP:NE1	2.20	0.56
1:B:60:LEU:HD13	1:B:223:TRP:NE1	2.20	0.56
1:B:91:THR:HG1	2:B:301:ARG:N	2.04	0.56
1:C:60:LEU:HD13	1:C:223:TRP:NE1	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ALA:CB	1:C:64:VAL:HG22	2.36	0.55
1:D:34:LYS:HD3	1:D:187:TYR:OH	2.07	0.54
1:B:51:ASP:HB2	1:B:240:LEU:HD21	1.90	0.54
1:C:123:ILE:HD12	1:C:129:LEU:CD1	2.38	0.53
1:D:189:ALA:O	1:D:190:LYS:CB	2.57	0.52
1:A:57:ALA:CB	1:A:64:VAL:HG22	2.39	0.52
1:D:117:LYS:HA	1:D:198:VAL:HG11	1.91	0.52
1:D:51:ASP:HB3	1:D:240:LEU:HD21	1.91	0.52
1:C:51:ASP:HB2	1:C:240:LEU:HD21	1.90	0.52
1:A:34:LYS:HG2	1:A:38:PHE:CG	2.44	0.51
1:D:182:SER:OG	1:D:183:PRO:HD3	2.10	0.51
1:A:154:LYS:O	1:D:161:GLU:OE2	2.28	0.50
1:D:91:THR:HG1	2:D:301:ARG:N	2.09	0.50
1:D:90:MET:HE2	1:D:96:ARG:HD3	1.95	0.48
1:A:51:ASP:HB3	1:A:240:LEU:HD21	1.95	0.48
1:A:107:MET:HG2	1:A:209:LEU:HD12	1.94	0.48
1:A:90:MET:HE2	1:A:96:ARG:HD3	1.96	0.48
1:B:112:THR:CG2	1:B:199:VAL:HG13	2.44	0.48
1:A:34:LYS:HG2	1:A:38:PHE:CD1	2.49	0.48
1:A:189:ALA:O	1:A:190:LYS:CB	2.61	0.47
1:D:107:MET:HG2	1:D:209:LEU:HD12	1.96	0.47
1:D:112:THR:CG2	1:D:199:VAL:HG13	2.45	0.47
1:A:22:ARG:NH1	1:A:26:ARG:NH1	2.63	0.47
1:C:90:MET:HE2	1:C:96:ARG:HD3	1.97	0.47
1:B:90:MET:HE2	1:B:96:ARG:HD3	1.97	0.46
1:D:39:LYS:HB3	1:D:45:TYR:CE1	2.51	0.46
1:B:34:LYS:NZ	1:D:219:GLU:CD	2.68	0.46
1:A:112:THR:CG2	1:A:199:VAL:HG13	2.46	0.46
1:C:202:GLU:CB	1:C:203:PRO:HD3	2.45	0.46
1:C:112:THR:CG2	1:C:199:VAL:HG13	2.46	0.46
1:C:107:MET:HG2	1:C:209:LEU:HD12	1.98	0.46
1:C:189:ALA:O	1:C:190:LYS:CB	2.64	0.45
1:B:108:THR:HG23	1:B:206:HIS:HB3	1.98	0.45
1:D:117:LYS:HA	1:D:198:VAL:CG1	2.46	0.45
1:A:91:THR:HG1	2:A:301:ARG:N	2.15	0.45
1:C:245:PHE:O	1:C:246:LYS:C	2.55	0.45
1:D:113:ILE:HB	1:D:200:VAL:HG13	1.99	0.44
1:D:60:LEU:CD1	1:D:223:TRP:NE1	2.81	0.44
1:A:34:LYS:CG	1:A:38:PHE:CG	3.01	0.44
1:B:22:ARG:NH1	1:B:26:ARG:NH1	2.66	0.43
1:A:204:PHE:O	1:A:205:THR:OG1	2.30	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:VAL:HG22	1:B:87:MET:HE3	2.00	0.43
1:C:113:ILE:HB	1:C:200:VAL:HG13	1.99	0.43
1:B:113:ILE:HB	1:B:200:VAL:HG13	1.99	0.43
1:B:30:ASP:HB2	2:B:301:ARG:HH22	1.83	0.42
1:C:27:VAL:HG22	1:C:87:MET:HE3	2.01	0.42
1:A:60:LEU:CD1	1:A:223:TRP:NE1	2.82	0.42
1:D:16:LEU:HD13	1:D:16:LEU:C	2.40	0.42
1:D:60:LEU:HB3	1:D:62:VAL:HG22	2.02	0.42
1:D:22:ARG:NH1	1:D:24:THR:O	2.53	0.42
1:A:181:ASP:OD2	2:A:301:ARG:N	2.53	0.42
1:C:114:LEU:HG	1:C:197:VAL:HG11	2.00	0.41
1:B:75:ILE:HD11	1:B:90:MET:CE	2.51	0.41
1:C:75:ILE:HD11	1:C:90:MET:CE	2.51	0.41
1:D:27:VAL:HG22	1:D:87:MET:HE3	2.01	0.41
1:A:201:ASP:O	1:A:203:PRO:HD3	2.21	0.41
1:C:60:LEU:HB3	1:C:62:VAL:HG22	2.02	0.41
1:D:75:ILE:HD11	1:D:90:MET:CE	2.51	0.40
1:A:75:ILE:HD11	1:A:90:MET:CE	2.52	0.40
1:B:60:LEU:HB3	1:B:62:VAL:HG22	2.03	0.40
1:C:143:THR:HG23	2:C:301:ARG:O	2.22	0.40

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	225/247 (91%)	211 (94%)	12 (5%)	2 (1%)	17	35
1	B	221/247 (90%)	211 (96%)	9 (4%)	1 (0%)	29	52
1	C	225/247 (91%)	213 (95%)	11 (5%)	1 (0%)	34	57
1	D	220/247 (89%)	211 (96%)	9 (4%)	0	100	100
All	All	891/988 (90%)	846 (95%)	41 (5%)	4 (0%)	34	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	ALA
1	B	196	ALA
1	C	202	GLU
1	A	204	PHE

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	184/209 (88%)	170 (92%)	14 (8%)	13	26
1	B	177/209 (85%)	165 (93%)	12 (7%)	16	32
1	C	171/209 (82%)	160 (94%)	11 (6%)	17	35
1	D	176/209 (84%)	165 (94%)	11 (6%)	18	36
All	All	708/836 (85%)	660 (93%)	48 (7%)	16	32

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	41	LYS
1	A	60	LEU
1	A	126	PHE
1	A	131	LYS
1	A	146	GLN
1	A	158	ARG
1	A	169	GLU
1	A	182	SER
1	A	195	LEU
1	A	198	VAL
1	A	201	ASP
1	A	236	THR
1	A	240	LEU
1	B	52	LEU
1	B	60	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	80	THR
1	B	131	LYS
1	B	136	VAL
1	B	140	LEU
1	B	182	SER
1	B	195	LEU
1	B	200	VAL
1	B	205	THR
1	B	236	THR
1	B	240	LEU
1	C	52	LEU
1	C	60	LEU
1	C	129	LEU
1	C	136	VAL
1	C	140	LEU
1	C	182	SER
1	C	198	VAL
1	C	200	VAL
1	C	205	THR
1	C	236	THR
1	C	240	LEU
1	D	25	LEU
1	D	52	LEU
1	D	60	LEU
1	D	127	GLU
1	D	131	LYS
1	D	136	VAL
1	D	140	LEU
1	D	158	ARG
1	D	161	GLU
1	D	200	VAL
1	D	236	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	ARG	B	301	-	7,11,11	0.80	1 (14%)	6,13,13	0.44	0
2	ARG	C	301	-	7,11,11	0.53	0	6,13,13	0.36	0
2	ARG	A	301	-	7,11,11	0.27	0	6,13,13	0.56	0
2	ARG	D	301	-	7,11,11	0.47	0	6,13,13	0.56	0

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	ARG	B	301	-	-	0/7/11/11	-
2	ARG	C	301	-	-	0/7/11/11	-
2	ARG	A	301	-	-	1/7/11/11	-
2	ARG	D	301	-	-	0/7/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ARG	CA-N	2.00	1.51	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ARG	NE-CD-CG-CB

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	ARG	2	0
2	C	301	ARG	2	0
2	A	301	ARG	2	0
2	D	301	ARG	1	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	229/247 (92%)	0.06	1 (0%) 92 91	18, 30, 58, 74	0
1	B	227/247 (91%)	0.38	13 (5%) 23 18	23, 42, 77, 111	0
1	C	229/247 (92%)	0.56	15 (6%) 18 13	34, 55, 90, 144	0
1	D	225/247 (91%)	0.25	9 (4%) 38 31	19, 40, 84, 102	0
All	All	910/988 (92%)	0.31	38 (4%) 36 29	18, 42, 81, 144	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	ILE	6.6
1	C	121	ASP	6.3
1	B	204	PHE	6.2
1	C	198	VAL	5.5
1	C	204	PHE	5.2
1	B	121	ASP	4.8
1	B	201	ASP	4.6
1	B	123	ILE	4.2
1	D	118	ASP	4.1
1	C	122	LYS	3.9
1	D	198	VAL	3.9
1	C	119	ASN	3.8
1	C	120	ALA	3.7
1	C	43	GLY	3.7
1	B	41	LYS	3.5
1	C	72	ASP	3.3
1	B	122	LYS	3.2
1	B	125	SER	3.1
1	B	200	VAL	3.0
1	D	121	ASP	2.8
1	B	242	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	132	PRO	2.5
1	D	126	PHE	2.5
1	C	200	VAL	2.4
1	B	133	ASP	2.4
1	A	197	VAL	2.4
1	D	237	TYR	2.3
1	B	98	LYS	2.3
1	B	44	GLN	2.2
1	C	42	ASN	2.2
1	C	67	VAL	2.2
1	D	199	VAL	2.2
1	C	176	ASP	2.1
1	D	13	ALA	2.1
1	C	233	LYS	2.1
1	C	197	VAL	2.1
1	D	205	THR	2.0
1	B	33	TYR	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 monosaccharides 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. 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
2	ARG	C	301	12/12	0.95	0.22	41,43,45,47	0
2	ARG	B	301	12/12	0.96	0.18	20,23,26,29	0
2	ARG	D	301	12/12	0.97	0.13	17,17,18,19	0
2	ARG	A	301	12/12	0.99	0.15	7,7,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.