



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:44 pm GMT

PDB ID : 2C3E
Title : The bovine mitochondrial ADP-ATP carrier
Authors : Nury, H.; Dahout-Gonzalez, C.; Trezeguet, V.; Lauquin, G.; Brandolin, G.;
Pebay-Peyroula, E.
Deposited on : 2005-10-06
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (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

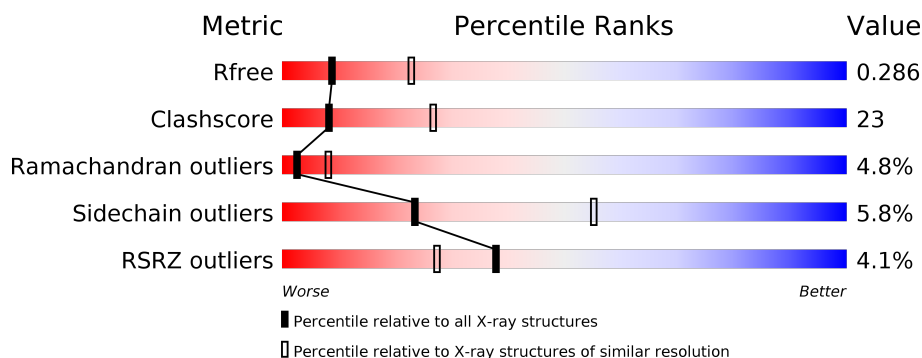
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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. 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	297	<div> <div>4%</div> <div>56%</div> <div>37%</div> <div>5%</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	CXT	A	401	X	-	-	-

2 Entry composition [i](#)

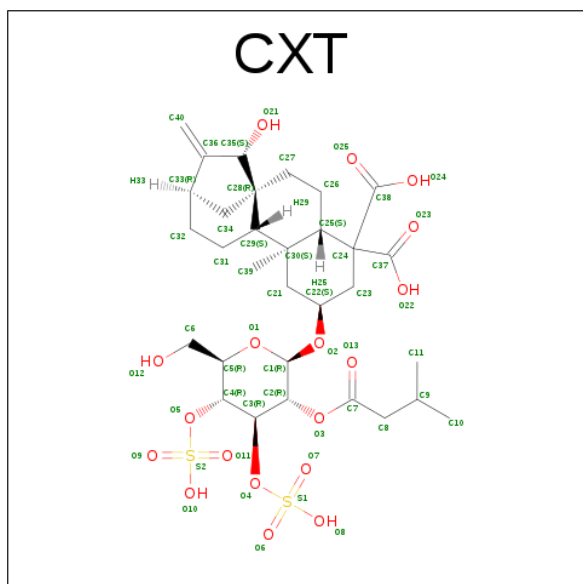
There are 3 unique types of molecules in this entry. The entry contains 2515 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ADP/ATP TRANSLOCASE 1.

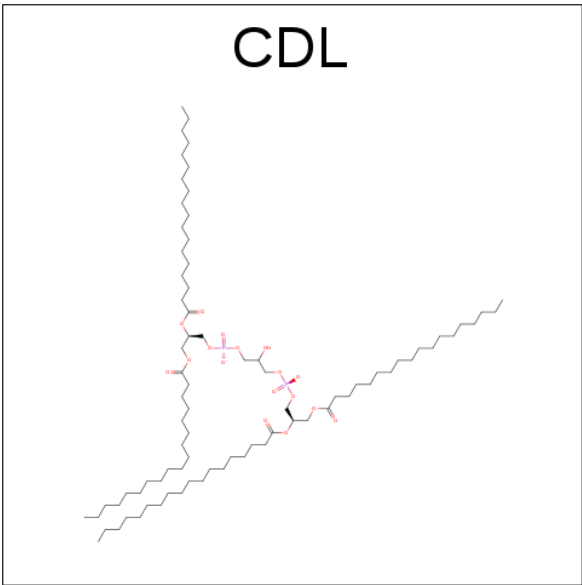
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	2266	1467	394	394	11	0	0	0

- Molecule 2 is CARBOXYATRACTYLOSIDE (three-letter code: CXT) (formula: $C_{31}H_{46}O_{18}S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	51	31	18	2	0	0

- Molecule 3 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			62	45	15	2		
3	A	1	Total	C	O	P	0	0
			55	36	17	2		
3	A	1	Total	C	O	P	0	0
			81	62	17	2		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	76.25Å 110.75Å 89.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 23.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (25.00-2.80) 98.0 (23.87-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.281 0.250 , 0.286	Depositor DCC
R_{free} test set	460 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 83.8	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	0.93	EDS
Total number of atoms	2515	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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

5.1 Standard geometry

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

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	0.47	0/2318	0.65	0/3128

There are no bond length outliers.

There are no bond angle outliers.

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	2266	0	2276	118	0
2	A	51	0	40	0	0
3	A	198	0	234	8	0
All	All	2515	0	2550	118	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 23.

All (118) 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:43:GLN:HE21	1:A:144:VAL:HG12	1.17	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLN:NE2	1:A:144:VAL:HG12	1.77	1.00
1:A:264:GLU:HB3	1:A:268:ALA:HB2	1.58	0.84
1:A:178:VAL:HG21	1:A:233:VAL:CG2	2.14	0.78
1:A:240:GLN:HE21	1:A:240:GLN:N	1.81	0.77
1:A:9:LYS:HD3	1:A:12:LEU:HD12	1.67	0.76
1:A:202:PRO:C	1:A:204:PRO:HD2	2.07	0.75
1:A:208:HIS:O	1:A:209:ILE:HG23	1.88	0.73
1:A:74:LEU:O	1:A:77:VAL:HG22	1.90	0.72
1:A:204:PRO:HG2	1:A:206:ASN:HB3	1.70	0.71
1:A:67:LEU:N	1:A:67:LEU:HD12	2.08	0.69
1:A:67:LEU:HD12	1:A:67:LEU:H	1.56	0.69
1:A:157:GLY:O	1:A:161:THR:HG23	1.93	0.68
1:A:204:PRO:C	1:A:206:ASN:H	1.96	0.68
1:A:44:ILE:HG22	1:A:49:GLN:HG2	1.75	0.68
1:A:38:GLN:HE22	1:A:50:TYR:H	1.41	0.67
1:A:176:PHE:HB3	3:A:802:CDL:HA32	1.76	0.67
1:A:273:ALA:O	1:A:277:VAL:HG23	1.93	0.67
1:A:30:ARG:HH22	1:A:64:GLN:HE22	1.43	0.66
1:A:264:GLU:HB3	1:A:268:ALA:CB	2.27	0.65
1:A:289:LEU:O	1:A:292:GLU:HG2	1.97	0.65
1:A:30:ARG:HH22	1:A:64:GLN:NE2	1.95	0.65
1:A:43:GLN:HE22	1:A:144:VAL:H	1.45	0.63
1:A:178:VAL:HG21	1:A:233:VAL:HG21	1.78	0.63
1:A:212:SER:O	1:A:215:ILE:HG22	1.99	0.63
1:A:31:VAL:HG21	1:A:57:VAL:HG12	1.80	0.62
1:A:51:LYS:HD3	1:A:55:ASP:OD2	2.00	0.62
1:A:250:TYR:HE2	1:A:259:LYS:HB2	1.65	0.61
1:A:6:SER:O	1:A:7:PHE:HB2	2.00	0.60
1:A:131:TYR:HB3	1:A:132:PRO:HD3	1.84	0.59
1:A:290:TYR:O	1:A:292:GLU:N	2.36	0.59
1:A:38:GLN:NE2	1:A:49:GLN:HA	2.19	0.58
1:A:285:PHE:O	1:A:289:LEU:HD13	2.04	0.57
1:A:233:VAL:O	1:A:237:MET:HG2	2.03	0.57
1:A:208:HIS:ND1	1:A:209:ILE:HG12	2.18	0.57
1:A:44:ILE:CG2	1:A:49:GLN:HG2	2.34	0.57
1:A:237:MET:SD	1:A:256:CYS:HB2	2.44	0.57
1:A:272:GLY:N	3:A:801:CDL:OB4	2.35	0.57
1:A:164:PHE:C	1:A:166:SER:H	2.08	0.56
1:A:203:ASP:N	1:A:204:PRO:CD	2.69	0.56
1:A:147:GLY:C	1:A:149:ALA:H	2.08	0.56
1:A:194:TYR:HD1	1:A:219:VAL:HG11	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:H	1:A:67:LEU:CD1	2.19	0.56
1:A:130:VAL:HB	1:A:133:LEU:HD12	1.89	0.55
1:A:202:PRO:C	1:A:204:PRO:CD	2.75	0.55
1:A:48:LYS:HB3	1:A:48:LYS:NZ	2.21	0.55
1:A:21:SER:O	1:A:25:VAL:HG22	2.06	0.54
1:A:12:LEU:O	1:A:16:VAL:HG23	2.08	0.54
1:A:215:ILE:O	1:A:219:VAL:HG23	2.09	0.53
1:A:285:PHE:O	1:A:288:VAL:HB	2.09	0.52
1:A:94:TYR:OH	3:A:802:CDL:H192	2.10	0.52
1:A:250:TYR:CE2	1:A:259:LYS:HB2	2.44	0.51
1:A:50:TYR:CD2	1:A:56:CYS:HA	2.45	0.51
1:A:31:VAL:HG11	1:A:53:ILE:HG23	1.91	0.51
1:A:32:LYS:HG3	1:A:276:ASN:HB2	1.93	0.51
1:A:147:GLY:O	1:A:149:ALA:N	2.44	0.51
1:A:53:ILE:HG13	3:A:801:CDL:HB22	1.93	0.51
1:A:26:ALA:N	1:A:27:PRO:CD	2.74	0.50
1:A:127:LEU:O	1:A:129:PHE:N	2.45	0.50
1:A:252:GLY:H	1:A:255:ASP:HB3	1.77	0.49
1:A:204:PRO:C	1:A:206:ASN:N	2.65	0.49
1:A:258:ARG:HG2	1:A:258:ARG:HH11	1.78	0.49
1:A:2:ASP:O	1:A:3:GLN:HG3	2.13	0.49
1:A:37:VAL:HG11	1:A:235:ARG:HB3	1.95	0.48
1:A:222:VAL:O	1:A:226:VAL:HG23	2.13	0.48
1:A:289:LEU:H	1:A:289:LEU:CD1	2.26	0.48
1:A:54:ILE:O	1:A:58:VAL:HB	2.13	0.48
1:A:255:ASP:O	1:A:259:LYS:HD3	2.13	0.48
1:A:145:GLY:HA3	1:A:150:GLN:O	2.13	0.47
1:A:153:PHE:CD2	1:A:159:CYS:HA	2.48	0.47
1:A:164:PHE:C	1:A:166:SER:N	2.67	0.47
1:A:239:MET:C	1:A:240:GLN:HE21	2.16	0.47
1:A:64:GLN:HG2	1:A:145:GLY:O	2.14	0.47
1:A:254:VAL:O	1:A:258:ARG:HB2	2.14	0.47
1:A:43:GLN:HE22	1:A:144:VAL:N	2.13	0.47
1:A:264:GLU:OE1	1:A:268:ALA:HB1	2.15	0.47
1:A:38:GLN:HE22	1:A:49:GLN:HA	1.78	0.47
1:A:267:LYS:O	1:A:268:ALA:C	2.52	0.46
1:A:247:ASP:O	1:A:249:MET:N	2.48	0.46
1:A:74:LEU:HD12	3:A:800:CDL:HA21	1.98	0.46
1:A:44:ILE:HG22	1:A:45:SER:O	2.16	0.46
1:A:250:TYR:HE2	1:A:259:LYS:CB	2.26	0.46
1:A:21:SER:HA	1:A:286:VAL:HG11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD13	1:A:156:LEU:HD23	1.98	0.45
1:A:32:LYS:HD3	1:A:32:LYS:C	2.38	0.44
1:A:267:LYS:C	1:A:269:PHE:N	2.70	0.44
1:A:67:LEU:N	1:A:67:LEU:CD1	2.76	0.44
1:A:132:PRO:O	1:A:135:PHE:HB3	2.19	0.43
1:A:147:GLY:C	1:A:149:ALA:N	2.70	0.43
1:A:78:ILE:O	1:A:82:PRO:HD2	2.18	0.43
1:A:71:ARG:HG2	1:A:140:LEU:O	2.19	0.43
1:A:240:GLN:HE21	1:A:240:GLN:CA	2.32	0.43
1:A:247:ASP:O	1:A:248:ILE:C	2.57	0.43
1:A:108:PHE:C	1:A:108:PHE:CD2	2.92	0.42
1:A:208:HIS:HB3	1:A:211:VAL:HG23	2.01	0.42
1:A:19:ALA:HB1	3:A:800:CDL:H751	2.01	0.42
1:A:240:GLN:NE2	1:A:240:GLN:CA	2.82	0.42
1:A:80:TYR:CZ	1:A:84:GLN:HG3	2.53	0.42
1:A:229:PRO:HG3	1:A:270:PHE:CE1	2.55	0.42
1:A:73:ASN:O	1:A:76:ASN:N	2.52	0.42
1:A:289:LEU:N	1:A:289:LEU:CD1	2.82	0.42
1:A:285:PHE:CZ	1:A:289:LEU:HD11	2.54	0.42
1:A:130:VAL:O	1:A:131:TYR:C	2.58	0.41
1:A:240:GLN:NE2	1:A:240:GLN:N	2.59	0.41
1:A:277:VAL:O	1:A:281:MET:HG3	2.20	0.41
1:A:16:VAL:HA	3:A:800:CDL:H792	2.02	0.41
1:A:43:GLN:HB2	1:A:43:GLN:HE21	1.61	0.41
1:A:274:TRP:HB2	3:A:801:CDL:HB61	2.02	0.41
1:A:38:GLN:HE22	1:A:50:TYR:N	2.13	0.41
1:A:247:ASP:O	1:A:249:MET:HG3	2.21	0.41
1:A:95:LYS:O	1:A:99:LEU:HB2	2.20	0.41
1:A:267:LYS:HB2	1:A:267:LYS:HE2	1.92	0.41
1:A:207:VAL:O	1:A:208:HIS:C	2.59	0.40
1:A:79:ARG:HD2	1:A:130:VAL:HG21	2.04	0.40
1:A:32:LYS:O	1:A:36:GLN:HB2	2.21	0.40
1:A:127:LEU:O	1:A:128:CYS:C	2.59	0.40
1:A:127:LEU:HD22	1:A:131:TYR:HD1	1.86	0.40
1:A:279:ARG:NH1	1:A:280:GLY:HA2	2.36	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	291/297 (98%)	247 (85%)	30 (10%)	14 (5%)	2 8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	7	PHE
1	A	207	VAL
1	A	209	ILE
1	A	248	ILE
1	A	291	ASP
1	A	79	ARG
1	A	128	CYS
1	A	148	ALA
1	A	260	ILE
1	A	206	ASN
1	A	203	ASP
1	A	5	LEU
1	A	208	HIS

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	225/234 (96%)	212 (94%)	13 (6%)	23 55

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	10	ASP
1	A	34	LEU
1	A	64	GLN
1	A	74	LEU
1	A	102	VAL
1	A	105	HIS
1	A	137	ARG
1	A	153	PHE
1	A	194	TYR
1	A	235	ARG
1	A	240	GLN
1	A	289	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	36	GLN
1	A	38	GLN
1	A	39	HIS
1	A	43	GLN
1	A	64	GLN
1	A	73	ASN
1	A	96	GLN
1	A	158	ASN
1	A	240	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	CXT	A	401	-	51,55,55	3.22	22 (43%)	64,89,89	2.98	21 (32%)
3	CDL	A	800	-	61,61,99	0.69	0	62,72,111	1.05	5 (8%)
3	CDL	A	801	-	54,54,99	0.80	2 (3%)	56,66,111	1.18	7 (12%)
3	CDL	A	802	-	80,80,99	0.71	3 (3%)	82,92,111	0.90	5 (6%)

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	CXT	A	401	-	1/1/20/20	0/24/120/120	0/3/5/5
3	CDL	A	800	-	-	0/70/70/110	0/0/0/0
3	CDL	A	801	-	-	0/65/65/110	0/0/0/0
3	CDL	A	802	-	-	0/91/91/110	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	CXT	O21-C35	-4.99	1.32	1.42
2	A	401	CXT	O2-C1	-3.82	1.31	1.41
2	A	401	CXT	O13-C7	-3.11	1.13	1.22
2	A	401	CXT	O4-C3	-2.52	1.41	1.46
2	A	401	CXT	O5-C4	-2.10	1.41	1.46
3	A	802	CDL	OA8-CA7	2.02	1.39	1.33
2	A	401	CXT	C8-C7	2.05	1.54	1.50
2	A	401	CXT	O1-C1	2.24	1.47	1.41
2	A	401	CXT	C23-C22	2.25	1.56	1.51
3	A	802	CDL	CB3-CB4	2.32	1.57	1.50
3	A	802	CDL	CA3-CA4	2.33	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	CDL	CB3-CB4	2.34	1.57	1.50
3	A	801	CDL	OA8-CA7	2.39	1.40	1.33
2	A	401	CXT	C21-C30	2.48	1.58	1.54
2	A	401	CXT	C27-C26	2.60	1.59	1.53
2	A	401	CXT	C28-C35	2.90	1.64	1.56
2	A	401	CXT	O2-C22	3.79	1.50	1.44
2	A	401	CXT	C26-C25	4.50	1.61	1.53
2	A	401	CXT	C39-C30	4.51	1.62	1.54
2	A	401	CXT	C24-C37	5.44	1.60	1.50
2	A	401	CXT	C28-C29	6.14	1.68	1.55
2	A	401	CXT	C31-C29	6.45	1.64	1.53
2	A	401	CXT	C40-C36	6.47	1.45	1.32
2	A	401	CXT	C24-C38	6.53	1.62	1.50
2	A	401	CXT	C24-C25	6.62	1.69	1.58
2	A	401	CXT	O3-C7	6.63	1.53	1.34
2	A	401	CXT	C30-C25	8.34	1.70	1.56

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CXT	O2-C22-C23	-7.26	86.37	107.83
2	A	401	CXT	O3-C7-C8	-6.59	99.12	111.47
2	A	401	CXT	C26-C25-C30	-4.87	105.74	110.95
2	A	401	CXT	C23-C24-C25	-3.82	101.64	110.32
3	A	801	CDL	CA6-CA4-CA3	-3.34	104.33	111.86
2	A	401	CXT	C39-C30-C21	-3.25	103.87	108.90
2	A	401	CXT	O3-C2-C3	-2.77	102.70	108.23
3	A	801	CDL	O1-C1-CA2	-2.62	99.69	109.34
2	A	401	CXT	O2-C1-O1	-2.59	104.40	110.70
2	A	401	CXT	C21-C30-C25	-2.42	105.02	107.83
3	A	801	CDL	CB6-CB4-CB3	-2.26	106.76	111.86
3	A	802	CDL	OB6-CB5-OB7	-2.24	118.09	123.68
3	A	800	CDL	OB6-CB5-OB7	-2.23	118.11	123.68
2	A	401	CXT	C3-C4-C5	-2.20	105.85	110.55
2	A	401	CXT	O1-C5-C6	-2.17	101.20	106.41
3	A	802	CDL	O1-C1-CA2	-2.03	101.85	109.34
3	A	801	CDL	OB6-CB5-C51	2.00	115.72	111.55
2	A	401	CXT	O2-C1-C2	2.01	113.20	109.07
3	A	800	CDL	C52-C51-CB5	2.12	121.32	113.58
3	A	802	CDL	C52-C51-CB5	2.13	121.37	113.58
3	A	800	CDL	OB8-CB6-CB4	2.21	114.21	108.66
3	A	802	CDL	OB6-CB5-C51	2.29	116.30	111.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CXT	C6-C5-C4	2.30	119.51	113.24
2	A	401	CXT	C32-C33-C36	2.32	114.53	110.48
3	A	800	CDL	OB6-CB5-C51	2.38	116.50	111.55
3	A	801	CDL	C52-C51-CB5	2.40	122.36	113.58
3	A	801	CDL	CB4-OB6-CB5	2.44	123.65	117.88
2	A	401	CXT	C39-C30-C25	2.76	118.04	112.94
2	A	401	CXT	C1-C2-C3	2.90	116.69	110.74
2	A	401	CXT	O3-C2-C1	2.99	115.36	108.47
2	A	401	CXT	C1-O1-C5	3.03	119.42	113.72
2	A	401	CXT	O3-C7-O13	3.23	131.72	123.68
3	A	802	CDL	OB8-CB6-CB4	3.45	117.33	108.66
3	A	801	CDL	OB8-CB6-CB4	3.72	117.99	108.66
3	A	800	CDL	OA6-CA4-CA3	4.23	115.26	105.88
2	A	401	CXT	O12-C6-C5	4.25	125.65	111.34
2	A	401	CXT	C3-O4-S1	6.59	131.64	118.97
2	A	401	CXT	O2-C22-C21	14.67	151.20	107.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	CXT	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	CDL	3	0
3	A	801	CDL	3	0
3	A	802	CDL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	293/297 (98%)	0.35	12 (4%) 38 27	51, 82, 153, 185	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	13.0
1	A	2	ASP	6.6
1	A	200	MET	4.3
1	A	134	ASP	4.0
1	A	169	LEU	3.1
1	A	138	THR	3.0
1	A	235	ARG	3.0
1	A	201	LEU	2.6
1	A	288	VAL	2.5
1	A	3	GLN	2.5
1	A	244	LYS	2.4
1	A	85	ALA	2.3

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	CDL	A	802	81/100	0.66	0.35	1.84	139,139,139,139	0
3	CDL	A	801	55/100	0.87	0.25	1.61	91,91,91,91	0
3	CDL	A	800	62/100	0.79	0.30	1.34	111,111,111,111	0
2	CXT	A	401	51/51	0.91	0.23	-0.02	89,89,89,89	0

6.5 Other polymers

There are no such residues in this entry.