



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 02:17 PM JST

PDB ID : 7EHL
EMDB ID : EMD-31142
Title : Cryo-EM structure of human ABCB8 transporter in nucleotide binding state
Authors : Li, S.J.; Yang, X.; Shen, Y.Q.
Deposited on : 2021-03-29
Resolution : Not provided

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

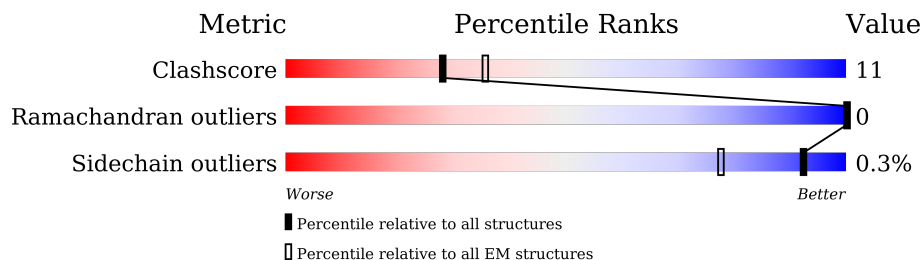
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	678	 68% 15% 17%
1	B	678	 67% 16% 17%

2 Entry composition [i](#)

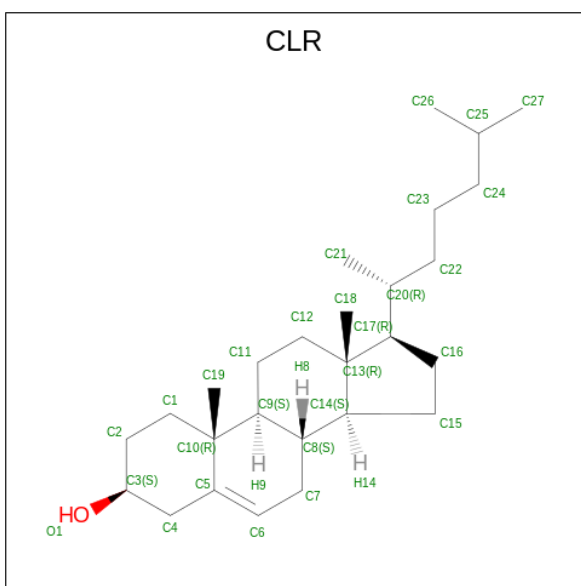
There are 4 unique types of molecules in this entry. The entry contains 8048 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Mitochondrial potassium channel ATP-binding subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	563	Total 3936	C 2488	N 694	O 737	S 17	0	0
1	B	563	Total 3936	C 2488	N 694	O 737	S 17	0	0

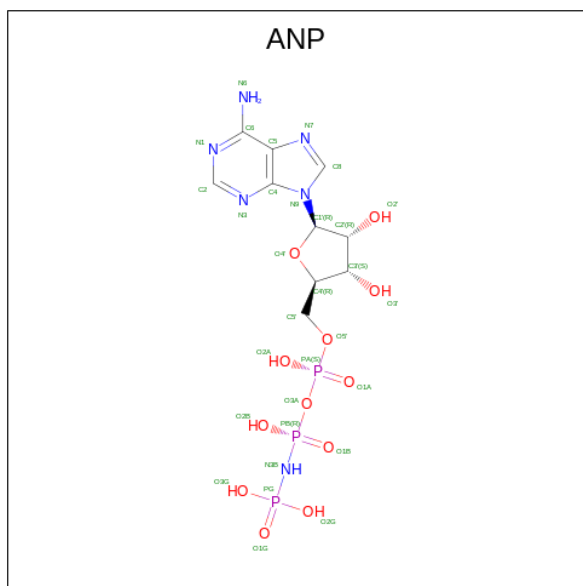
- Molecule 2 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	Total 56	C 54	O 2	0
2	A	1	Total 56	C 54	O 2	0
2	B	1	Total 56	C 54	O 2	0
2	B	1	Total 56	C 54	O 2	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
3	A	1	31	10	6	12	3	0
3	B	1	31	10	6	12	3	0

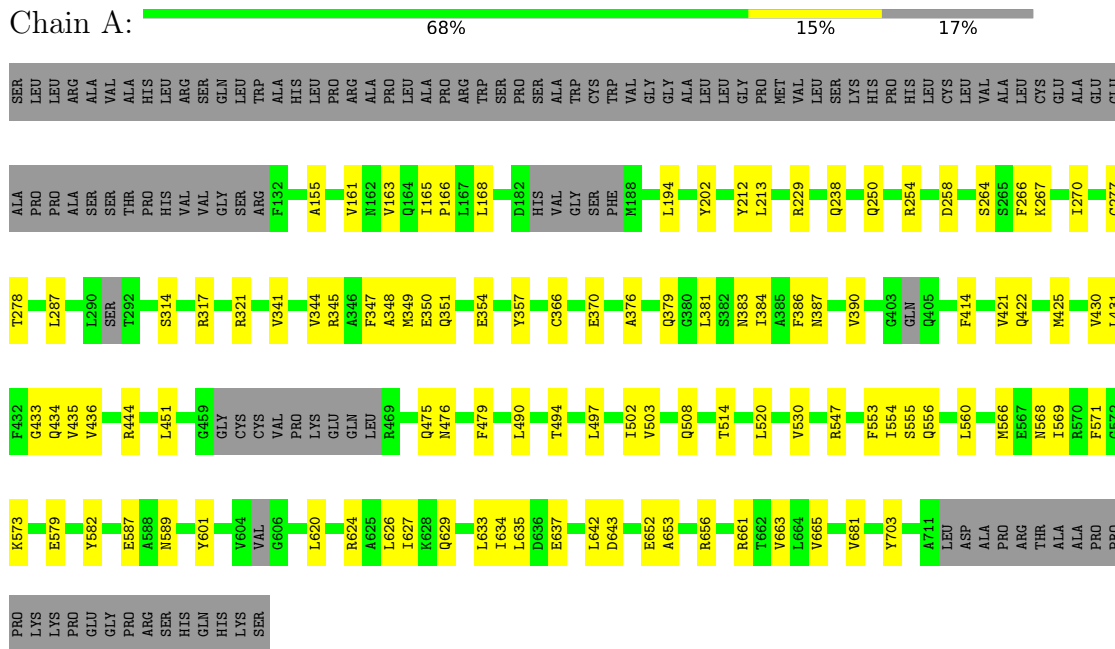
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0
4	B	1	1	1	0

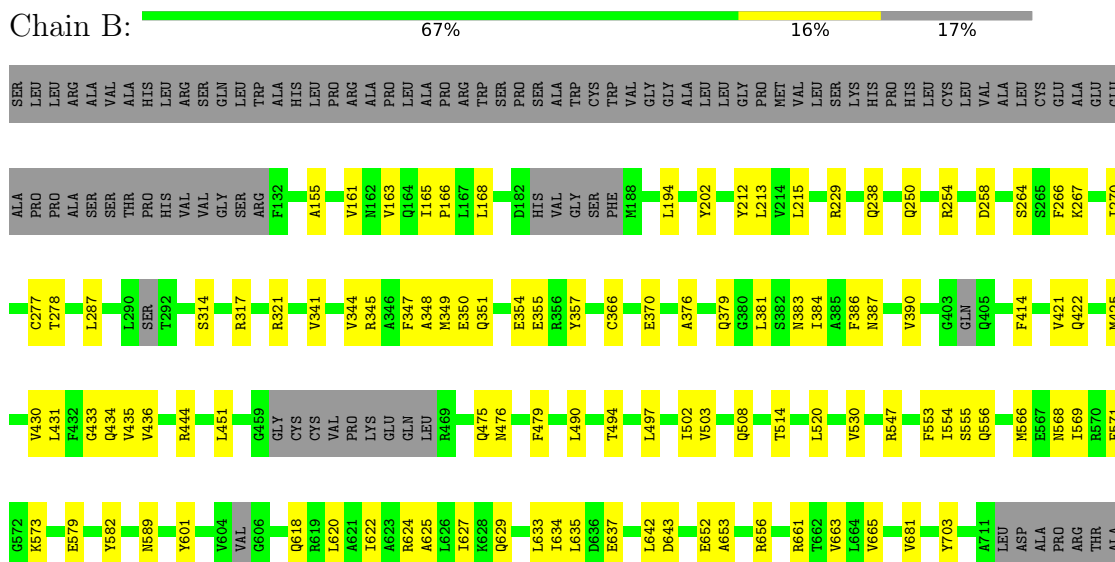
3 Residue-property plots [i](#)

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. 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. 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: Mitochondrial potassium channel ATP-binding subunit



- Molecule 1: Mitochondrial potassium channel ATP-binding subunit



ALA
PRO
PRO
PRO
LYS
LYS
PRO
GLU
GLY
PRO
ARG
SER
HIS
GLN
HIS
LYS
SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43131	Depositor
Resolution determination method	Not provided	
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, CLR

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	0.28	0/3991	0.52	0/5431
1	B	0.28	0/3991	0.52	0/5431
All	All	0.28	0/7982	0.52	0/10862

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 [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	3936	0	3657	87	0
1	B	3936	0	3657	86	0
2	A	56	0	92	5	0
2	B	56	0	92	5	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	8048	0	7522	165	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 11.

All (165) 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:B:568:ASN:OD1	1:B:624:ARG:NH2	1.71	1.24
1:A:569:ILE:HD11	1:A:620:LEU:HD12	1.33	1.06
1:A:633:LEU:HB2	1:A:663:VAL:HG12	1.10	1.04
1:A:569:ILE:HD11	1:A:620:LEU:CD1	1.95	0.96
1:A:633:LEU:HB2	1:A:663:VAL:CG1	2.04	0.85
1:A:633:LEU:CB	1:A:663:VAL:HG12	2.04	0.83
1:B:351:GLN:HA	1:B:351:GLN:HE21	1.48	0.78
1:A:569:ILE:CD1	1:A:620:LEU:HD12	2.15	0.76
1:A:568:ASN:OD1	1:A:624:ARG:NH2	2.17	0.76
1:A:560:LEU:HD11	1:A:620:LEU:CD2	2.16	0.76
1:B:573:LYS:NZ	1:B:627:ILE:HG22	2.00	0.75
1:B:589:ASN:OD1	1:B:656:ARG:NH2	2.22	0.73
1:A:589:ASN:OD1	1:A:656:ARG:NH2	2.22	0.72
1:B:573:LYS:HZ1	1:B:627:ILE:HG22	1.55	0.71
1:A:202:TYR:CE2	1:B:384:ILE:HD12	2.27	0.70
1:A:384:ILE:HD12	1:B:202:TYR:CE2	2.27	0.69
1:A:573:LYS:NZ	1:A:627:ILE:HG22	2.07	0.68
1:A:383:ASN:O	1:B:202:TYR:OH	2.12	0.68
1:A:569:ILE:CD1	1:A:620:LEU:CD1	2.71	0.68
1:A:629:GLN:HB3	1:A:661:ARG:HH21	1.58	0.68
1:A:202:TYR:OH	1:B:383:ASN:O	2.12	0.68
1:B:629:GLN:HB3	1:B:661:ARG:HH21	1.58	0.68
1:A:387:ASN:HB2	1:B:202:TYR:CZ	2.30	0.67
1:A:202:TYR:CZ	1:B:387:ASN:HB2	2.30	0.67
1:B:351:GLN:HA	1:B:351:GLN:NE2	2.08	0.67
1:A:476:ASN:H	1:A:494:THR:HG22	1.60	0.66
1:B:476:ASN:H	1:B:494:THR:HG22	1.60	0.65
1:A:653:ALA:HA	1:A:656:ARG:HE	1.63	0.63
1:A:479:PHE:H	1:A:490:LEU:HB2	1.64	0.62
1:A:508:GLN:N	1:A:508:GLN:OE1	2.33	0.62
1:B:479:PHE:H	1:B:490:LEU:HB2	1.64	0.62
1:B:653:ALA:HA	1:B:656:ARG:HE	1.63	0.62
1:A:560:LEU:HD11	1:A:620:LEU:HD22	1.82	0.62
1:B:421:VAL:O	1:B:425:MET:HG2	2.00	0.62
1:A:421:VAL:O	1:A:425:MET:HG2	2.00	0.60
1:B:508:GLN:N	1:B:508:GLN:OE1	2.33	0.59
1:A:155:ALA:HB2	1:A:212:TYR:CE1	2.37	0.59
1:B:155:ALA:HB2	1:B:212:TYR:CE1	2.37	0.58
1:A:387:ASN:HB2	1:B:202:TYR:OH	2.04	0.58
1:A:202:TYR:OH	1:B:387:ASN:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:GLN:O	1:B:355:GLU:OE1	2.22	0.57
1:A:314:SER:HA	1:A:317:ARG:HE	1.70	0.57
1:B:314:SER:HA	1:B:317:ARG:HE	1.70	0.56
1:A:587:GLU:OE1	1:A:626:LEU:HD13	2.06	0.56
1:B:475:GLN:HB3	1:B:530:VAL:HG12	1.90	0.53
1:A:250:GLN:OE1	1:A:254:ARG:NH2	2.42	0.53
1:A:502:ILE:HD12	1:A:663:VAL:CG2	2.38	0.53
1:A:381:LEU:HA	1:A:384:ILE:HG22	1.91	0.53
1:A:579:GLU:HA	1:A:582:TYR:HD2	1.74	0.53
1:B:579:GLU:HA	1:B:582:TYR:HD2	1.74	0.53
1:A:264:SER:HA	1:A:267:LYS:NZ	2.24	0.52
1:A:475:GLN:HB3	1:A:530:VAL:HG12	1.90	0.52
1:B:350:GLU:O	1:B:354:GLU:HG3	2.09	0.52
1:B:381:LEU:HA	1:B:384:ILE:HG22	1.91	0.52
1:B:264:SER:HA	1:B:267:LYS:NZ	2.24	0.52
1:B:514:THR:OG1	3:B:1003:ANP:O1A	2.27	0.52
1:A:161:VAL:O	1:A:165:ILE:HG12	2.10	0.52
1:B:258:ASP:OD1	1:B:444:ARG:NH2	2.29	0.52
1:B:502:ILE:HD12	1:B:663:VAL:CG1	2.40	0.52
1:A:213:LEU:HD21	1:B:379:GLN:NE2	2.25	0.52
1:A:350:GLU:O	1:A:354:GLU:HG3	2.09	0.52
1:A:379:GLN:NE2	1:B:213:LEU:HD21	2.25	0.52
1:A:573:LYS:HZ3	1:A:627:ILE:HG22	1.74	0.51
1:A:514:THR:OG1	3:A:902:ANP:O1A	2.27	0.51
1:B:554:ILE:HD11	1:B:625:ALA:CB	2.41	0.51
1:A:560:LEU:CD1	1:A:620:LEU:CD2	2.87	0.50
1:B:351:GLN:HE21	1:B:351:GLN:CA	2.14	0.50
1:A:266:PHE:CZ	1:A:270:ILE:HD11	2.46	0.50
1:B:266:PHE:CZ	1:B:270:ILE:HD11	2.46	0.50
1:B:553:PHE:HE1	1:B:555:SER:HB2	1.75	0.50
1:A:553:PHE:HE1	1:A:555:SER:HB2	1.75	0.50
1:A:566:MET:HB2	1:A:601:TYR:HB3	1.94	0.50
1:B:161:VAL:O	1:B:165:ILE:HG12	2.10	0.50
1:B:566:MET:HB2	1:B:601:TYR:HB3	1.94	0.50
1:B:250:GLN:OE1	1:B:254:ARG:NH2	2.42	0.50
1:A:520:LEU:H	1:A:520:LEU:HD23	1.78	0.49
1:B:556:GLN:HB3	1:B:637:GLU:HB3	1.95	0.48
1:A:556:GLN:HB3	1:A:637:GLU:HB3	1.95	0.48
1:B:520:LEU:HD11	1:B:634:ILE:HD11	1.96	0.48
1:B:238:GLN:NE2	1:B:451:LEU:HB2	2.29	0.48
1:A:238:GLN:NE2	1:A:451:LEU:HB2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ILE:CD1	1:A:620:LEU:HD11	2.44	0.47
1:A:547:ARG:NH1	1:B:345:ARG:O	2.47	0.47
1:B:568:ASN:CG	1:B:624:ARG:HH21	2.04	0.47
1:A:652:GLU:O	1:A:656:ARG:HG2	2.15	0.47
1:A:163:VAL:O	1:A:166:PRO:HD2	2.15	0.47
2:B:1001:CLR:H183	2:B:1001:CLR:H20	1.75	0.47
1:A:520:LEU:HD11	1:A:634:ILE:HD11	1.96	0.47
1:B:163:VAL:O	1:B:166:PRO:HD2	2.15	0.47
1:A:264:SER:HA	1:A:267:LYS:HZ2	1.78	0.47
1:B:351:GLN:NE2	1:B:351:GLN:CA	2.73	0.46
1:A:386:PHE:O	1:A:390:VAL:HG23	2.15	0.46
1:B:633:LEU:CB	1:B:663:VAL:HG23	2.45	0.46
1:B:345:ARG:HA	1:B:345:ARG:HD2	1.76	0.46
1:B:520:LEU:HD23	1:B:520:LEU:H	1.78	0.46
1:B:386:PHE:O	1:B:390:VAL:HG23	2.15	0.46
1:B:652:GLU:O	1:B:656:ARG:HG2	2.15	0.45
2:B:1001:CLR:H222	2:B:1001:CLR:H162	1.77	0.45
1:B:341:VAL:HA	1:B:344:VAL:HG12	1.99	0.45
2:A:903:CLR:H222	2:A:903:CLR:H162	1.77	0.45
1:A:345:ARG:O	1:B:547:ARG:NH1	2.47	0.45
1:A:229:ARG:HA	1:B:357:TYR:HE2	1.82	0.44
2:B:1001:CLR:H211	2:B:1001:CLR:H231	1.77	0.44
1:A:341:VAL:HA	1:A:344:VAL:HG12	1.99	0.44
1:A:345:ARG:HA	1:A:345:ARG:HD2	1.76	0.44
1:B:238:GLN:HE22	1:B:451:LEU:HB2	1.82	0.44
1:A:642:LEU:HD12	1:A:643:ASP:O	2.17	0.44
1:B:642:LEU:HD12	1:B:643:ASP:O	2.17	0.44
1:B:571:PHE:CD2	1:B:624:ARG:HD3	2.53	0.44
1:A:238:GLN:HE22	1:A:451:LEU:HB2	1.82	0.43
1:A:357:TYR:HE2	1:B:229:ARG:HA	1.82	0.43
2:A:901:CLR:H183	2:A:901:CLR:H20	1.76	0.43
2:A:903:CLR:H211	2:A:903:CLR:H231	1.77	0.43
1:A:573:LYS:HZ1	1:A:627:ILE:HG22	1.80	0.43
1:A:479:PHE:HB3	1:A:490:LEU:HD13	2.01	0.43
1:A:587:GLU:OE1	1:A:626:LEU:CD1	2.66	0.43
1:B:573:LYS:HZ3	1:B:627:ILE:HG22	1.81	0.43
1:A:381:LEU:O	1:A:384:ILE:HG22	2.18	0.43
1:B:264:SER:HA	1:B:267:LYS:HZ2	1.84	0.43
1:B:381:LEU:O	1:B:384:ILE:HG22	2.18	0.43
1:B:168:LEU:HD11	1:B:194:LEU:HD12	2.00	0.43
1:B:497:LEU:HD22	1:B:503:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:903:CLR:H232	1:B:422:GLN:HE21	1.85	0.42
1:B:277:CYS:SG	1:B:278:THR:N	2.93	0.42
2:B:1002:CLR:H183	2:B:1002:CLR:H20	1.76	0.42
1:A:430:VAL:HG12	1:A:434:GLN:OE1	2.19	0.42
1:B:433:GLY:HA2	1:B:436:VAL:HG12	2.02	0.42
1:B:502:ILE:CD1	1:B:663:VAL:HG12	2.49	0.42
1:A:168:LEU:HD11	1:A:194:LEU:HD12	2.00	0.42
1:A:277:CYS:SG	1:A:278:THR:N	2.93	0.42
1:B:479:PHE:HB3	1:B:490:LEU:HD13	2.01	0.42
1:B:376:ALA:O	1:B:379:GLN:HG3	2.20	0.42
1:B:569:ILE:HD11	1:B:620:LEU:HD13	2.02	0.42
1:A:349:MET:HE3	1:B:573:LYS:HA	2.01	0.42
1:B:553:PHE:O	1:B:554:ILE:HD13	2.20	0.42
1:B:633:LEU:HB2	1:B:663:VAL:HG23	2.02	0.42
1:A:347:PHE:O	1:A:348:ALA:HB3	2.20	0.42
1:A:431:LEU:O	1:A:435:VAL:HG23	2.19	0.42
1:A:433:GLY:HA2	1:A:436:VAL:HG12	2.02	0.42
1:B:430:VAL:HG12	1:B:434:GLN:OE1	2.19	0.42
1:B:618:GLN:O	1:B:622:ILE:HG13	2.20	0.42
1:A:351:GLN:O	1:A:354:GLU:N	2.53	0.41
1:B:431:LEU:O	1:B:435:VAL:HG23	2.19	0.41
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.89	0.41
1:A:502:ILE:CD1	1:A:663:VAL:HG22	2.50	0.41
1:A:422:GLN:HE21	2:B:1001:CLR:H232	1.85	0.41
1:A:553:PHE:O	1:A:554:ILE:HD13	2.20	0.41
1:B:635:LEU:HB2	1:B:665:VAL:HG23	2.03	0.41
1:A:497:LEU:HD22	1:A:503:VAL:HG21	2.01	0.41
1:B:287:LEU:HD22	1:B:414:PHE:HD1	1.86	0.41
2:A:903:CLR:H183	2:A:903:CLR:H20	1.75	0.41
1:A:635:LEU:HB2	1:A:665:VAL:HG23	2.03	0.41
1:B:681:VAL:HG21	1:B:703:TYR:HB2	2.03	0.41
1:A:287:LEU:HD22	1:A:414:PHE:HD1	1.86	0.41
1:A:568:ASN:O	1:A:571:PHE:HB2	2.21	0.41
1:A:573:LYS:HA	1:B:349:MET:HE3	2.02	0.41
1:A:258:ASP:OD1	1:A:444:ARG:NH2	2.29	0.40
1:A:376:ALA:O	1:A:379:GLN:HG3	2.20	0.40
1:B:347:PHE:O	1:B:348:ALA:HB3	2.20	0.40
1:B:366:CYS:O	1:B:370:GLU:OE1	2.39	0.40
1:B:314:SER:HA	1:B:317:ARG:NE	2.35	0.40
1:B:568:ASN:O	1:B:571:PHE:HB2	2.21	0.40
1:A:366:CYS:O	1:A:370:GLU:OE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:VAL:HG21	1:A:703:TYR:HB2	2.03	0.40
1:A:579:GLU:HA	1:A:582:TYR:CD2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	551/678 (81%)	532 (97%)	19 (3%)	0	100	100
1	B	551/678 (81%)	532 (97%)	19 (3%)	0	100	100
All	All	1102/1356 (81%)	1064 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	356/552 (64%)	355 (100%)	1 (0%)	92	92
1	B	356/552 (64%)	355 (100%)	1 (0%)	92	92
All	All	712/1104 (64%)	710 (100%)	2 (0%)	92	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	ARG
1	B	321	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	351	GLN

5.3.3 RNA [i](#)

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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	CLR	B	1002	-	31,31,31	3.48	13 (41%)	48,48,48	2.60	14 (29%)
3	ANP	A	902	4	29,33,33	3.51	17 (58%)	31,52,52	1.41	4 (12%)
3	ANP	B	1003	4	29,33,33	3.51	17 (58%)	31,52,52	1.41	4 (12%)
2	CLR	A	901	-	31,31,31	3.48	13 (41%)	48,48,48	2.60	14 (29%)
2	CLR	B	1001	-	31,31,31	3.48	13 (41%)	48,48,48	2.59	14 (29%)
2	CLR	A	903	-	31,31,31	3.48	13 (41%)	48,48,48	2.59	14 (29%)

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	CLR	B	1002	-	-	4/10/68/68	0/4/4/4
3	ANP	A	902	4	-	5/14/38/38	0/3/3/3
3	ANP	B	1003	4	-	5/14/38/38	0/3/3/3
2	CLR	A	901	-	-	4/10/68/68	0/4/4/4
2	CLR	B	1001	-	-	6/10/68/68	0/4/4/4
2	CLR	A	903	-	-	6/10/68/68	0/4/4/4

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	903	CLR	C6-C5	10.58	1.56	1.33
2	B	1001	CLR	C6-C5	10.58	1.56	1.33
2	A	901	CLR	C6-C5	10.52	1.56	1.33
2	B	1002	CLR	C6-C5	10.52	1.56	1.33
3	A	902	ANP	O4'-C1'	-7.59	1.30	1.41
3	B	1003	ANP	O4'-C1'	-7.59	1.30	1.41
3	A	902	ANP	C3'-C4'	-7.29	1.34	1.53
3	B	1003	ANP	C3'-C4'	-7.29	1.34	1.53
2	A	901	CLR	C16-C15	6.92	1.73	1.54
2	B	1002	CLR	C16-C15	6.92	1.73	1.54
2	A	903	CLR	C16-C15	6.80	1.72	1.54
2	B	1001	CLR	C16-C15	6.80	1.72	1.54
3	A	902	ANP	PB-O3A	6.64	1.67	1.59
3	B	1003	ANP	PB-O3A	6.64	1.67	1.59
3	A	902	ANP	O4'-C4'	6.48	1.59	1.45
3	B	1003	ANP	O4'-C4'	6.48	1.59	1.45
2	A	901	CLR	C20-C17	-6.37	1.43	1.54
2	B	1002	CLR	C20-C17	-6.37	1.43	1.54
2	A	903	CLR	C20-C17	-6.10	1.43	1.54
2	B	1001	CLR	C20-C17	-6.10	1.43	1.54
2	A	903	CLR	C13-C17	6.02	1.66	1.55
2	B	1001	CLR	C13-C17	6.02	1.66	1.55
2	A	903	CLR	C8-C9	5.78	1.64	1.53
2	B	1001	CLR	C8-C9	5.78	1.64	1.53
2	A	901	CLR	C8-C9	5.72	1.64	1.53
2	B	1002	CLR	C8-C9	5.72	1.64	1.53
2	A	901	CLR	C13-C17	5.56	1.65	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	CLR	C13-C17	5.56	1.65	1.55
3	A	902	ANP	PG-O1G	5.35	1.54	1.46
3	B	1003	ANP	PG-O1G	5.35	1.54	1.46
2	A	901	CLR	C15-C14	5.07	1.64	1.54
2	B	1002	CLR	C15-C14	5.07	1.64	1.54
2	A	903	CLR	C12-C11	5.04	1.64	1.53
2	B	1001	CLR	C12-C11	5.04	1.64	1.53
2	A	901	CLR	C12-C11	5.00	1.64	1.53
2	B	1002	CLR	C12-C11	5.00	1.64	1.53
2	A	903	CLR	C15-C14	4.94	1.64	1.54
2	B	1001	CLR	C15-C14	4.94	1.64	1.54
3	A	902	ANP	PB-O1B	3.82	1.52	1.46
3	B	1003	ANP	PB-O1B	3.82	1.52	1.46
3	A	902	ANP	PB-O2B	-3.81	1.46	1.56
3	B	1003	ANP	PB-O2B	-3.81	1.46	1.56
3	A	902	ANP	PG-N3B	3.72	1.73	1.63
3	B	1003	ANP	PG-N3B	3.72	1.73	1.63
2	A	901	CLR	C7-C6	3.60	1.57	1.50
2	B	1002	CLR	C7-C6	3.60	1.57	1.50
2	A	903	CLR	C7-C6	3.57	1.57	1.50
2	B	1001	CLR	C7-C6	3.57	1.57	1.50
3	A	902	ANP	C2-N1	-3.56	1.27	1.33
3	B	1003	ANP	C2-N1	-3.56	1.27	1.33
3	A	902	ANP	PB-N3B	3.52	1.72	1.63
3	B	1003	ANP	PB-N3B	3.52	1.72	1.63
3	A	902	ANP	O2'-C2'	-3.40	1.35	1.43
3	B	1003	ANP	O2'-C2'	-3.40	1.35	1.43
3	A	902	ANP	O3'-C3'	3.18	1.50	1.43
3	B	1003	ANP	O3'-C3'	3.18	1.50	1.43
3	A	902	ANP	PG-O3G	-2.99	1.48	1.56
3	B	1003	ANP	PG-O3G	-2.99	1.48	1.56
3	A	902	ANP	C6-N6	2.76	1.44	1.34
3	B	1003	ANP	C6-N6	2.76	1.44	1.34
2	A	903	CLR	C4-C5	2.57	1.57	1.51
2	B	1001	CLR	C4-C5	2.57	1.57	1.51
2	A	901	CLR	C4-C5	2.55	1.57	1.51
2	B	1002	CLR	C4-C5	2.55	1.57	1.51
3	A	902	ANP	C4-N3	-2.38	1.32	1.35
3	B	1003	ANP	C4-N3	-2.38	1.32	1.35
2	A	903	CLR	C7-C8	2.27	1.57	1.53
2	B	1001	CLR	C7-C8	2.27	1.57	1.53
2	A	901	CLR	C7-C8	2.27	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	CLR	C7-C8	2.27	1.57	1.53
2	A	901	CLR	C4-C3	2.19	1.56	1.52
2	B	1002	CLR	C4-C3	2.19	1.56	1.52
3	A	902	ANP	C2'-C1'	2.12	1.57	1.53
3	B	1003	ANP	C2'-C1'	2.12	1.57	1.53
2	A	903	CLR	C4-C3	2.11	1.55	1.52
2	B	1001	CLR	C4-C3	2.11	1.55	1.52
2	A	901	CLR	C22-C20	2.10	1.59	1.54
2	B	1002	CLR	C22-C20	2.10	1.59	1.54
2	A	903	CLR	C11-C9	-2.10	1.50	1.53
2	B	1001	CLR	C11-C9	-2.10	1.50	1.53
3	A	902	ANP	C5-C4	-2.09	1.35	1.40
3	B	1003	ANP	C5-C4	-2.09	1.35	1.40
2	A	903	CLR	C22-C20	2.09	1.59	1.54
2	B	1001	CLR	C22-C20	2.09	1.59	1.54
2	A	901	CLR	C11-C9	-2.08	1.50	1.53
2	B	1002	CLR	C11-C9	-2.08	1.50	1.53

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	CLR	C4-C5-C6	-7.30	110.08	120.61
2	B	1002	CLR	C4-C5-C6	-7.30	110.08	120.61
2	A	903	CLR	C4-C5-C6	-7.25	110.15	120.61
2	B	1001	CLR	C4-C5-C6	-7.25	110.15	120.61
2	A	901	CLR	C10-C5-C6	-6.71	112.63	122.90
2	B	1002	CLR	C10-C5-C6	-6.71	112.63	122.90
2	A	903	CLR	C7-C6-C5	-6.71	112.69	125.06
2	B	1001	CLR	C7-C6-C5	-6.71	112.69	125.06
2	A	903	CLR	C10-C5-C6	-6.65	112.73	122.90
2	B	1001	CLR	C10-C5-C6	-6.65	112.73	122.90
2	A	901	CLR	C7-C6-C5	-6.64	112.82	125.06
2	B	1002	CLR	C7-C6-C5	-6.64	112.82	125.06
2	A	901	CLR	C13-C17-C20	-6.18	109.81	119.49
2	B	1002	CLR	C13-C17-C20	-6.18	109.81	119.49
2	A	903	CLR	C13-C17-C20	-5.18	111.38	119.49
2	B	1001	CLR	C13-C17-C20	-5.18	111.38	119.49
2	A	903	CLR	C17-C13-C14	5.10	106.11	100.07
2	B	1001	CLR	C17-C13-C14	5.10	106.11	100.07
3	A	902	ANP	N3-C2-N1	-4.37	121.85	128.68
3	B	1003	ANP	N3-C2-N1	-4.37	121.85	128.68
2	A	901	CLR	C12-C13-C14	4.31	113.96	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	CLR	C12-C13-C14	4.31	113.96	107.27
2	A	903	CLR	C4-C5-C10	-3.86	111.30	116.42
2	B	1001	CLR	C4-C5-C10	-3.86	111.30	116.42
2	A	901	CLR	C4-C5-C10	-3.81	111.36	116.42
2	B	1002	CLR	C4-C5-C10	-3.81	111.36	116.42
2	A	903	CLR	C18-C13-C12	-3.68	104.78	110.59
2	B	1001	CLR	C18-C13-C12	-3.68	104.78	110.59
2	A	901	CLR	C18-C13-C17	-3.62	104.95	111.71
2	B	1002	CLR	C18-C13-C17	-3.62	104.95	111.71
2	A	901	CLR	C17-C13-C14	3.55	104.27	100.07
2	B	1002	CLR	C17-C13-C14	3.55	104.27	100.07
2	A	901	CLR	C18-C13-C12	-3.53	105.01	110.59
2	B	1002	CLR	C18-C13-C12	-3.53	105.01	110.59
2	A	903	CLR	C18-C13-C17	-3.44	105.30	111.71
2	B	1001	CLR	C18-C13-C17	-3.44	105.30	111.71
2	A	903	CLR	C18-C13-C14	-3.37	105.42	111.71
2	B	1001	CLR	C18-C13-C14	-3.37	105.42	111.71
2	A	903	CLR	C12-C13-C17	3.36	121.60	116.57
2	B	1001	CLR	C12-C13-C17	3.36	121.60	116.57
2	A	901	CLR	C12-C13-C17	3.34	121.58	116.57
2	B	1002	CLR	C12-C13-C17	3.34	121.58	116.57
2	A	903	CLR	C12-C13-C14	3.25	112.32	107.27
2	B	1001	CLR	C12-C13-C14	3.25	112.32	107.27
2	A	901	CLR	C18-C13-C14	-3.19	105.76	111.71
2	B	1002	CLR	C18-C13-C14	-3.19	105.76	111.71
2	A	903	CLR	C19-C10-C9	-2.96	108.15	111.68
2	B	1001	CLR	C19-C10-C9	-2.96	108.15	111.68
2	A	901	CLR	C19-C10-C9	-2.86	108.27	111.68
2	B	1002	CLR	C19-C10-C9	-2.86	108.27	111.68
3	A	902	ANP	C3'-C2'-C1'	2.66	104.98	100.98
3	B	1003	ANP	C3'-C2'-C1'	2.66	104.98	100.98
2	A	903	CLR	C11-C9-C10	-2.54	109.73	113.08
2	B	1001	CLR	C11-C9-C10	-2.54	109.73	113.08
2	A	901	CLR	C21-C20-C17	-2.52	109.06	112.92
2	B	1002	CLR	C21-C20-C17	-2.52	109.06	112.92
2	A	901	CLR	C11-C9-C10	-2.42	109.89	113.08
2	B	1002	CLR	C11-C9-C10	-2.42	109.89	113.08
3	A	902	ANP	PB-O3A-PA	-2.42	124.11	132.62
3	B	1003	ANP	PB-O3A-PA	-2.42	124.11	132.62
3	A	902	ANP	C4-C5-N7	-2.31	106.99	109.40
3	B	1003	ANP	C4-C5-N7	-2.31	106.99	109.40
2	A	903	CLR	C16-C17-C13	2.13	106.41	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	CLR	C16-C17-C13	2.13	106.41	103.84

There are no chirality outliers.

All (30) torsion outliers are listed below:

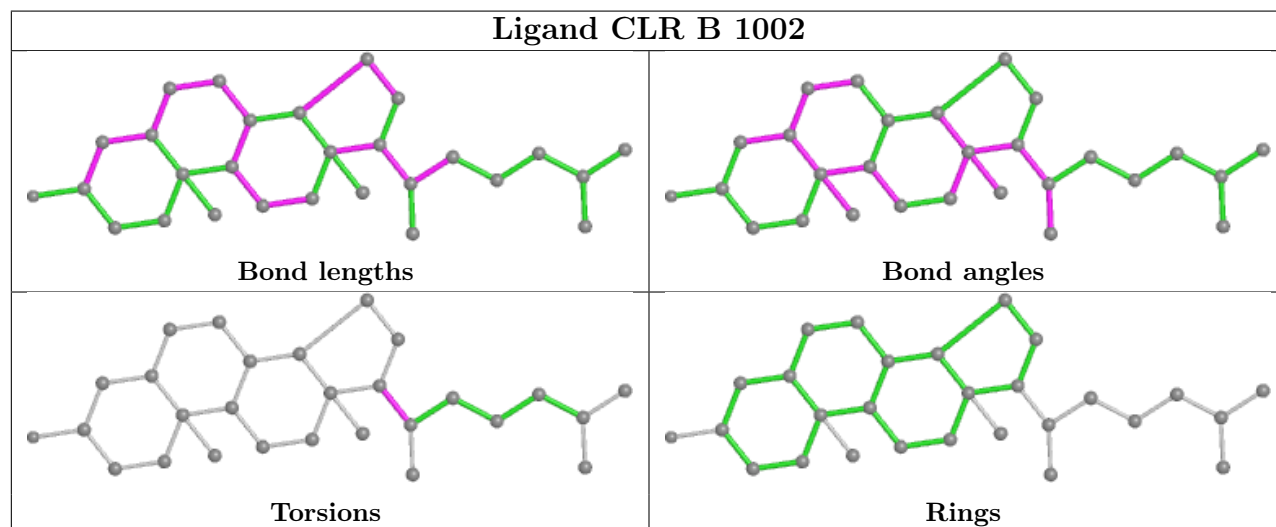
Mol	Chain	Res	Type	Atoms
2	A	901	CLR	C13-C17-C20-C21
2	B	1002	CLR	C13-C17-C20-C21
3	A	902	ANP	PG-N3B-PB-O1B
3	A	902	ANP	C5'-O5'-PA-O1A
3	A	902	ANP	C5'-O5'-PA-O2A
3	A	902	ANP	C5'-O5'-PA-O3A
3	B	1003	ANP	PG-N3B-PB-O1B
3	B	1003	ANP	C5'-O5'-PA-O1A
3	B	1003	ANP	C5'-O5'-PA-O2A
3	B	1003	ANP	C5'-O5'-PA-O3A
2	A	901	CLR	C16-C17-C20-C21
2	B	1002	CLR	C16-C17-C20-C21
2	A	901	CLR	C13-C17-C20-C22
2	B	1002	CLR	C13-C17-C20-C22
2	A	901	CLR	C16-C17-C20-C22
2	B	1002	CLR	C16-C17-C20-C22
2	A	903	CLR	C22-C23-C24-C25
2	B	1001	CLR	C22-C23-C24-C25
2	A	903	CLR	C13-C17-C20-C21
2	B	1001	CLR	C13-C17-C20-C21
2	A	903	CLR	C16-C17-C20-C21
2	B	1001	CLR	C16-C17-C20-C21
2	A	903	CLR	C13-C17-C20-C22
2	B	1001	CLR	C13-C17-C20-C22
2	A	903	CLR	C20-C22-C23-C24
2	B	1001	CLR	C20-C22-C23-C24
2	A	903	CLR	C16-C17-C20-C22
2	B	1001	CLR	C16-C17-C20-C22
3	A	902	ANP	C4'-C5'-O5'-PA
3	B	1003	ANP	C4'-C5'-O5'-PA

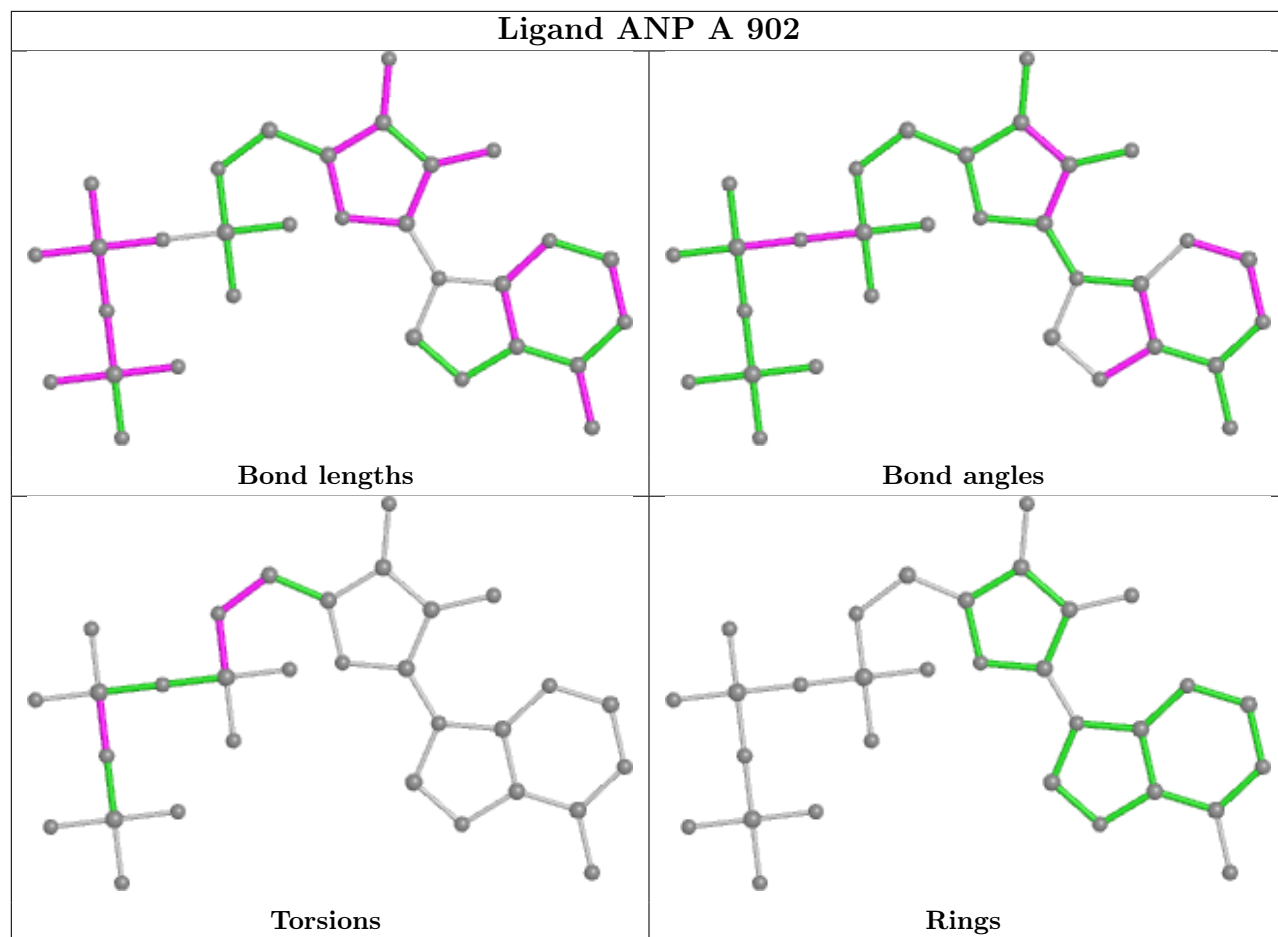
There are no ring outliers.

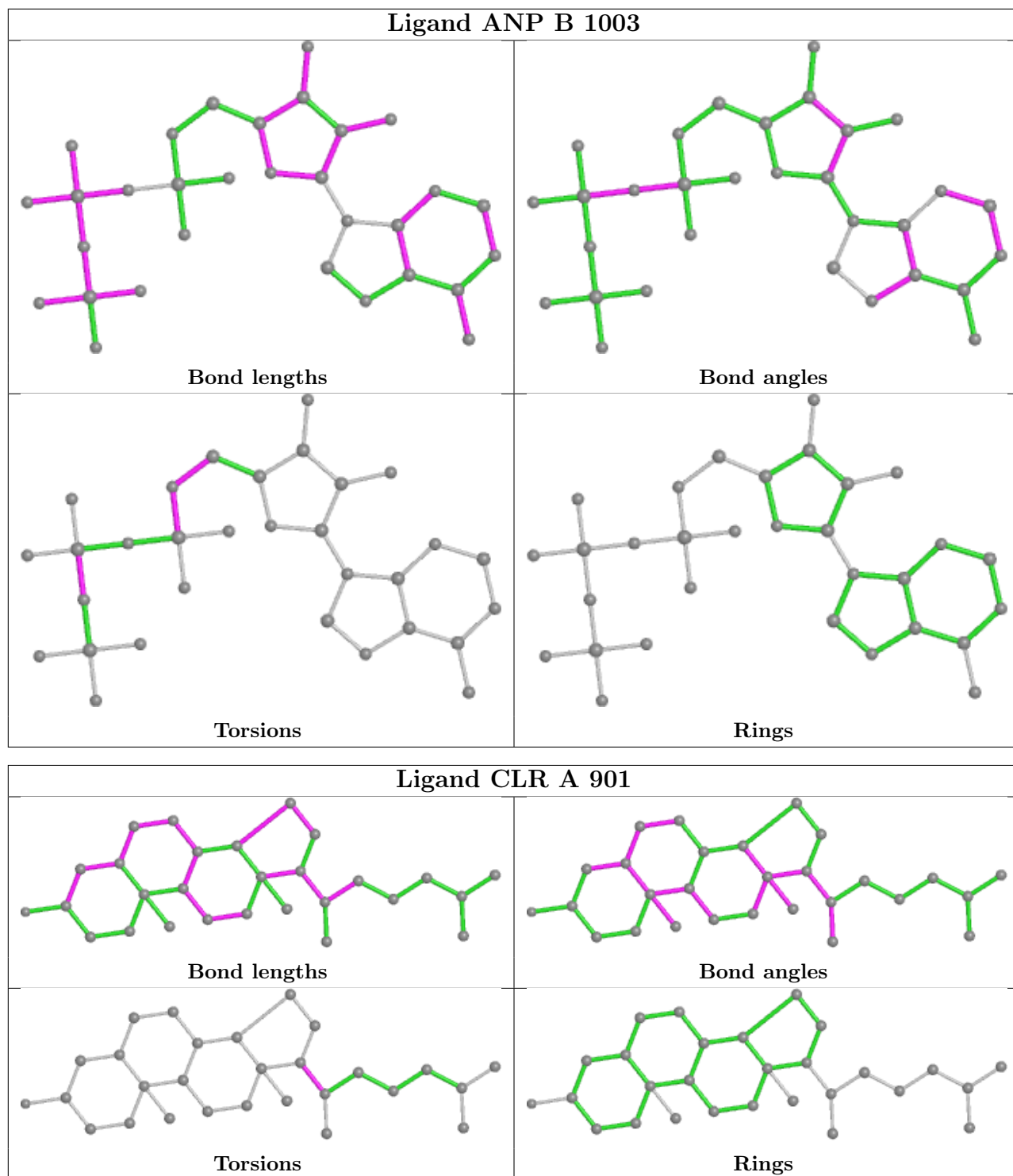
6 monomers are involved in 12 short contacts:

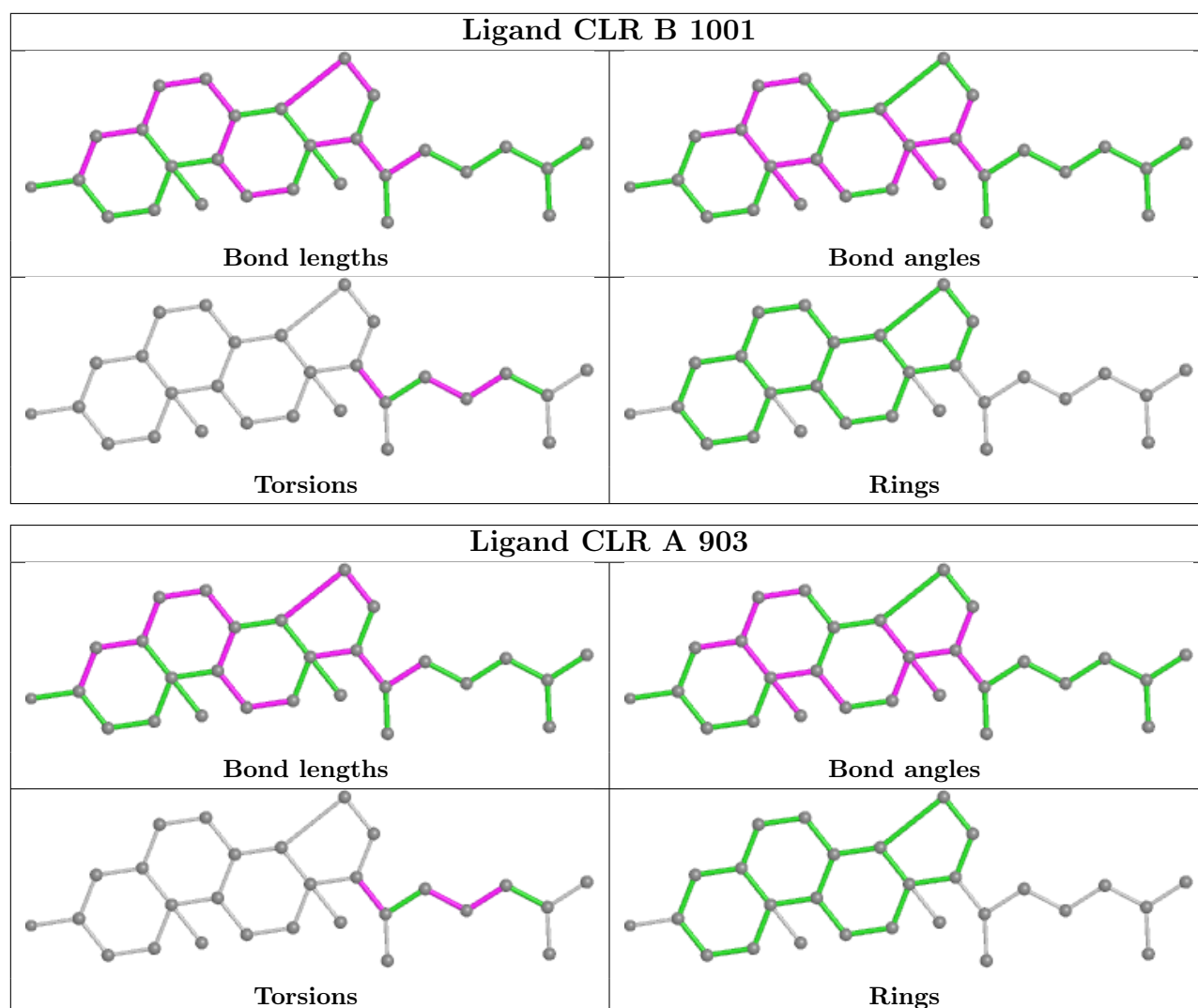
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	CLR	1	0
3	A	902	ANP	1	0
3	B	1003	ANP	1	0
2	A	901	CLR	1	0
2	B	1001	CLR	4	0
2	A	903	CLR	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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 Map visualisation

This section contains visualisations of the EMDB entry EMD-31142. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.